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ESTUARINE MODELING: AN ASSESSMENT

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27 Abstract

~~This report constitutes~~ a technical review and critical appraisal are presented of present techniques of water quality modeling as applied to estuaries. Various aspects of estuarine modeling are treated by a selection of scientists and engineers eminent in the field, and these essays are supplemented by discussions from technical conferences held during the course of the report's preparation. Topics discussed include mathematical models for estuarine hydrodynamics, water quality models of chemical and biological constituents, models of estuarine temperature structure, and the use of physical models in estuarine analysis. Also included is a review of solution techniques, viz. analog, digital and hybrid, a brief survey of estuarine biota and biological modeling, and a collection of case studies reviewing several estuarine modeling projects. Conclusions about the existing state of the art of estuarine modeling and recommendations for future research ~~by EPA~~ are summarized, ~~in the final chapter.~~ (EPA abstract)

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ESTUARINE MODELING: AN ASSESSMENT

Capabilities and Limitations for Resource Management and Pollution Control

Edited by

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ABSTRACT

This report constitutes a technical review and critical appraisal of present techniques of water quality modeling as applied to estuaries. Various aspects of estuarine modeling are treated by a selection of scientists and engineers eminent in the field, and these essays are supplemented by discussions from technical conferences held during the course of the report's preparation. Topics discussed include one-, two-, and three-dimensional mathematical models for estuarine hydrodynamics, water quality models of chemical and biological constitutents including DO, BOD, nitrogen forms, phytoplankton and general coupled reactants, models of estuarine temperature structure with special attention given the modeling of thermal discharges, and the principles and applicability of physical models in estuarine analysis. Also included is a review of solution techniques, viz. analog, digital and hybrid with a detailed discussion of finite-difference methods, a brief survey of estuarine biota and present biological modeling activities, and a collection of case studies reviewing several past estuarine modeling projects. Conclusions about the existing state of the art of estuarine modeling and recommendations for future research by EPA are advanced throughout the report and are summarized in the final chapter.

This report was submitted in fulfillment of Project No. 16070DZV between the Environmental Protection Agency and TRACOR, Inc., as part of the National Coastal Pollution Research Program.

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FOREWORD

The Water Quality Office of the Environmental Protection Agency has historically supported research and development efforts for estuarine models, and is continuing to do so. The purpose of this report is to provide a summary of presently available modeling methods used in studying the causes of estuarine pollution problems and pollution abatement alternatives.

This current project has been undertaken by the National Coastal Pollution Research Program as part of an overall mission to expand scientific understanding of the marine environment with respect to improvement and protection of marine water quality. This mission is achieved by fundamental and applied studies on (a) physical transport and dispersion, (b) biological, chemical and physical transformations and interactions, (c) water use damages, (d) restoration of degraded marine waters, and (e) conservation of resources associated with additions of heat and materials introduced from land, rivers, and the atmosphere.

The nature of estuarine water pollution problems demands consideration of solid wastes which, through land use and ocean disposal, contribute materials to the estuarine system. Airborne materials can contribute to oceanic pollution--which can in turn influence or add to existing estuarine concentrations. Estuaries act as a focal point for man's environmental ills, screening, as they do, wastes discharged to inland watersheds and fed by small portions of all the wastes accumulated in the oceans. With the establishment of the Environmental Protection Agency there now appears to be a framework for estuarine pollution control consistent with the physical dimensions of the problem.

It was decided a report of this nature would be most beneficial if it were prepared by a group of consultants and specialists with considerable experience with one or more modeling topics. To make sure this assessment was directed to the problems pollution control agencies were working on now and foresaw as impending problems, members of the Federal Water Quality Administration regional office technical staffs were included.

This report presents a discussion of capabilities and limitations of both mathematical and physical models, and of various solution techniques for the mathematical formulations. Based on first-hand experience and a critical review of published reports by the authors and participants, recommendations are made for research and development found necessary to overcome deficiencies in present methods and to provide effective methods for handling more complex problems in the future.

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PREFACE

It is appropriate to include here some prefatory remarks on what this report is and what it is not, along with something about how it came to be. The purpose of this report is to critically appraise the present state of the art of water quality modeling as applied to estuaries. This purpose subsumes the question of how well do we understand estuarine processes, and includes, further, the questions: how well can we predict these processes, how well need we predict them for water quality regulation and management, and how do we best get from where we are to where we need to be. The answers provided to these questions are not simple, as can be judged from the bulk of this volume, nor in many cases are they complete or even clearly defined. But this is a liability of attempting to obtain these answers, quickly enough to be useful, from such a young, complex and vital field.

Although in a sense this report constitutes a cataloging of models, it is not intended nor written to be a reference manual for the practicing engineer. Many of the arguments require an examination of fundamentals, and return therefore to derivations and basic developments. But assumed throughout is an at least superficial familiarity of the reader with estuarine processes and their representation. Neither is this report a disjoint collection of technical papers, but it is, rather, an organic sequence of essays on assigned topics written from a consistent point of view.

The basic plan by which this report was prepared was to retain a group of consultants with considerable experience and expertise in aspects of estuarine modeling, some of whom would author the report and some of whom would provide a critical review. Preparation of the report was coordinated insofar as the geographical distribution of the consultants permitted, and was augmented by two general conferences attended by the consultants and those individuals in the Water Quality Office of EPA with direct responsibility for the development or application of models. These conferences were truly conferential, in that their purpose was to discuss in as much technical depth as necessary the various aspects of the report and of water quality models in general. In addition, throughout its preparation this report was open for discussions of the contents and the inclusion of alternate viewpoints. The discussions, both formal and informal, therefore constitute an integral and substantial part of the report.

The project was formally initiated in June 1969 and the first conference was held within the month at St. John's College in Annapolis, Maryland. The purpose of the conference was to agree on the content and scope of the report and to select the principal authors. The Water Quality Office (then FWPCA) had submitted a suggested outline consisting of five chapters, (i) mathematical models, (ii) analog and hybrid models, (iii) hydraulic models, (iv) use of models in evaluating streamflow regulation, and (v) use of models in evaluating physiographic modifications, which exemplifies the primary concerns of FWPCA at the time. At this conference the federal programs in estuarine water quality modeling were reviewed, and the report outlined in essentially its present form. (At the beginning of this work, the responsible agency was the Federal Water Pollution Control Administration, which subsequently became the Federal Water Quality Administration and is now the Water Quality Office of the Environmental Protection Agency. The agency is therefore referred to variously as FWPCA, FWQA and EPA throughout the report.)

After careful consideration of the report's intended content, scope and objectives, the resources available for its preparation were apportioned in the following way: hydrodynamics 20%, water quality 20%, temperature 6%, physical models 10%, solution techniques 20%, case studies 10%, biological modeling 2%, critical review 12%. While in fact the consultants contributed more than their allotted time, this distribution does serve, however, to indicate the relative weight given the various topics.

The authors of this report are men whose varied activities and scholarly pursuits place a high demand on their time. With such contributors, printing deadlines are propositions of naive optimism. (Out of similar undertakings has grown many an eloquent lament for the editor who daily nurses an empty mailbox.) Although it was scheduled that the second conference be convened in September and the report completed in November, or at least by the end of the year, it was not until June of 1970 that the second conference met in Salishan Lodge at Gleneden Beach, Oregon, nearly a year after the first conference. At this conference, the nearly complete report was subjected to a thorough and wide-ranging discussion. Plans were made for modifications and additions to the text and for its completion.

Editorial policy for the report was somewhat variable. The individual chapters were only lightly edited. Although notations could be made uniform, duplication eliminated, and the chapters modified to conform to a consistent style, we felt that in doing so, more would be lost than gained, and that the overall value of the report would be greatest if the identity and individuality of each author's work were preserved. The discussions, in contrast, required heavy editing, as a precise rendering in print of spoken dialog is less a transcript than a transmogrification. The contents of Chapter IX and the discussions appended to each chapter have been freely rearranged to achieve a more useful organization. As a general rule, discussions which involve technical details or which are of specific pertinence to a particular chapter are placed following that chapter, while discussions of a more general or recommendatory nature are included in Chapter IX. In no instance, however, are statements separated from the discussion context in which they occurred.

A number of acknowledgements are in order. Foremost are due D. J. Baumgartner and R. J. Callaway of the National Coastal Pollution Research Program of EPA. Their interest in the work and their resoluteness in achieving the project objective are in large measure responsible for the quality of this report. We are grateful for their assistance and support throughout the project.

The assistance and cooperation of our firm TRACOR, Inc., during the project is gratefully acknowledged. Several of our associates here, especially R. J. Huston and J. P. Buckner (now with the Coastal Bend Regional Planning Commission, Corpus Christi), contributed their assistance throughout the study. We wish to thank T. A. Wastler (Estuarine and Oceanographic Programs Branch, EPA) for his interest and comments, and EPA scientists and engineers, Norbert Jaworski, Howard Harris, George Pence, Tom Gallagher, Ken Feigner and John Vlastelecia, for their individual assistance, particularly in the compilation of the case studies (Chapter VII). E. G. Fruh (University of Texas) and B. J. Copeland (North Carolina State University) read portions of Chapter VII and their reviews lead to many substantive improvements. We are grateful to Colonel Frank P. Bender, Director of the Galveston Bay Project, for permitting the use in Chapter VII of results from the Galveston Bay Project. Dr. Garbis H. Keulegan of the Waterways Experiments Station has followed the preparation of the report since its inception, although owing to other commitments he was unable to formally review the document. We are grateful to him for his comments and for his great interest in the project.

We appreciate receiving permission from the following publishers and authors to reproduce copyrighted material: the American Society of Civil Engineers for several figures in Chapters IV, V and VII which appeared in the Proceedings, McGraw-Hill Book Company for Figure 2.10 from Estuary and Coastline Hydrodynamics, the Water Pollution Control Federation for Figures 3.11 - 3.17 from the Journal Water Pollution Control Federation, the American Fisheries Society for the quotation of Prof. Hedgpeth in Chapter VIII from A Symposium on Estuarine Fisheries, Donald Watts and O. L. Loucks of the University of Wisconsin for Figure 8.1 from Models for Describing Exchanges Within Ecosystems, the Controller of Her Britannic Majesty's Stationery Office for the figures and tables in Chapter VII from Effects of Polluting Discharges on the Thames Estuary, and the Controller of H. M. Stationery Office and the authors A. L. H. Gameson and I. C. Hart for Figure 7.29 and Table 7.4 from "A Study of Pollution in the Thames Estuary" in Chemistry and Industry. The data in Figure 7.29 and Table 7.4 are those of the Greater London Council.

Finally, we wish to express our gratitude to the consultants, Drs. Dobbins, Edinger, Harder, Harleman, Ippen, Leendertse, O'Connor, Paulik, Pritchard, Rattray and Thomann, who retained their patience and generosity through the eighteen long months this report was in preparation. This is their report. Its value and its merits are due to their integrity, their industry, and their command of their fields.

G.H.W.
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Austin
November 1970

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CHAPTER I

INTRODUCTION

George H. Ward, Jr.
and
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Growing concern with the preservation of our water resources, particularly within the last decade, has precipitated the need for a balanced and astute management of these resources. Even disregarding the political intricacies, water quality management is an exceedingly difficult task. The difficulties arise from two essential facts. First, utilization of the resources of a natural waterbody is subject, almost universally, to conflicts among potential users, in that one use inherently delimits or excludes another. The problems are compounded since, typically, each potential use is of some socio-economic importance. Much, if not most, of the management task ultimately devolves to the resolution of these conflicts in a satisfactory manner. Secondly, the processes--hydrographic, chemical, biological--which operate in a waterbody are extremely complex and often poorly understood. Yet it is these processes upon which management decisions must be based.

The application of water quality models has proved to be a powerful technique in water resource management, as models can incorporate the complexity of the relevant processes in the waterbody into a utilitarian form for management consideration. Through the use of models both a diagnostic and predictive capability is provided, diagnostic in the sense of permitting the identification and isolation of specific factors affecting the water quality, and predictive, in permitting evaluation of future effects of proposed changes in the waterbody, its inputs, or its uses.

1. ESTUARIES

This report is concerned with water quality modeling as applied to a specific type of waterbody, the estuary. (The general features of estuarine hydrography, viz., the defining characteristics of estuaries, associated circulation patterns, physiography, etc., are well known and may be assumed ab initio. See, e.g., Pritchard 1952, Cameron and Pritchard 1963, Lauff 1967.) This apparently superficial circumscription perhaps deserves discussion.

Estuaries are, collectively, of singular importance. They are important biologically; in contradistinction to the nutrient-rich water-poor land and the water-rich nutrient-poor ocean, estuaries are typically both a nutrient-rich and water-rich environment, highly productive, constituting the prime habitat for a myriad of species and the nursery and spawning area for many more. Besides their biological significance, however, estuaries are of specific importance to man, as is evidenced by their propensity for stimulating urban development. Estuaries offer an accessibility to the sea, often with excellent shipping and harbor facilities, while the feeding rivers provide a source of freshwater for domestic and industrial use, as well as affording receiving water for municipal and industrial wastes.

Estuaries are similarly quite susceptible to pollution and degradative modifications in quality. They often receive excessive volumes of wastes both from peripheral discharges and from upstream discharges carried into the estuary by the inflows, and are often adversely influenced by upstream freshwater consumption. In addition to affecting the estuary's own delicate ecology, the effects of these practices may extend beyond the physiographic bounds of the estuary itself.

Besides these very pragmatic reasons for a concern with estuaries, the estuary per se poses modeling problems of extreme scope and complexity. Its hydrodynamics, for instance, are determined by the interaction of the tides from the ocean and the influx of fresh water from the rivers, modified by complicated boundary stresses due to the semi-enclosed physiography, and further altered--or even dominated, as in fjords--by gravitational circulations arising from density gradients. These factors, however, are sufficient to characterize only the transport of a specific constituent in the estuary: the various processes and reactions to which that constituent is subjected must be determined as well. These range from simple first-order kinetics to reactions which depend nonlinearly upon additional variables and are possibly linked with the biota.

It is evident therefore that estuaries, besides comprising a water resource of critical importance, present modeling problems of intrinsic difficulty. This report attempts to summarize these problems and assess present methods for their treatment. Although many of the topics discussed can find application as well in coastal zones, in streams and rivers, or in lakes, the discussions are inclined to those aspects fundamental to, or peculiar to, estuarine processes.

2. ESTUARINE MODELS

The meaning of the term "model" as used in this report is not precise, and, indeed, four distinct meanings of the word as employed with regard to estuarine water quality may be identified. It is appropriate here to indicate these usages in a somewhat pedestrian manner, avoiding any judgments on their adequacy or correctness as such judgments can entail a lengthy philosophical digression. (Recent considerations of the meaning and role of models in science may be found in, e.g., Nagel, Suppes and Tarski 1962.)

In the strictest sense, a model is a formalism: the mathematical expression of the relevant physical processes, e.g., the application of the principles of Newtonian fluid mechanics with approximations appropriate to an estuary. A different but related usage is that a model is a conceptual idealization or simplified representation of a physical process. The employment of such a model is usually motivated by tractability and is justified by the ability of the model to reproduce observed results, even though it is ultimately unfaithful to the basic physics. One example is the representation of the Reynolds flux of salinity $\langle u_i's' \rangle$ by a "model" involving the product of the mean salt gradient and an eddy diffusivity $-K \frac{\partial s}{\partial x_i}$. (Another example, but not related to estuaries, is the representation of surface effects in vapor-drop equilibria by a "model" of the surface of the drop as a distensible membrane of constant tension--viz., the surface tension--even though the surface is known to be a transition region of high density gradient.)

"Model" is also used to mean a simple (in some sense) analog of the real system. In estuarine studies, the most familiar example is, of course, the physical or hydraulic model, a highly distorted, small-scale reproduction of the estuary complete with freshwater inflows, a sump of ocean salinity, and mechanical tide generators. This use of the term could as well apply to a simulator consisting of electrical components, as described in Chapter VI.

Finally, a "model" may refer to a mathematical formulation (a "model" in either the first or second sense above) together with a solution technique for the variables of concern. This usage is implicit in the expressions "analog model" and "digital model," and may in some cases even refer to a specific computer program, such as DECS-III or the WRE Model (the "Orlob Model"). This usage, which has some obvious faults, does not enjoy general approval by scientists and engineers involved in estuarine water quality, but nevertheless has become more frequent in recent years, particularly on the administrative or program level.

In the following pages all four uses of the term can be noted, sometimes in almost confusing contiguity. Probably the only definition of "model" sufficiently general to encompass these variations in meaning is the (superficial) statement that an estuarine model is a technique or device for the representation of some property in an estuary.

The preponderance of present estuarine water quality models is concerned with the concentration or distribution of a constituent, property or parameter in the estuary. Accordingly, the processes represented in the model are generally classified as either transport processes or reaction processes. Transport processes are basically hydrodynamic and include advection, turbulent diffusion, and, when spatial averaging is involved, dispersion. Reaction processes encompass the sources and sinks to which the parameter is subjected and may be physical, chemical or biological, e.g., sedimentation and flocculation of organics, uptake of oxygen in biochemical degradation of wastes, coliform mortality, algae loss by zooplankton grazing, etc. The relative importance of transport processes and reaction processes obviously varies from estuary to estuary, and depends upon the parameter modeled as well as the required spatial and temporal refinement.

The question eventually arises in the development of an estuarine model as to whether all of the relevant processes in the estuary have been identified or correctly represented. Classically this is determined by model verification, the comparison of model predictions with empirical measurements. As might be expected in a state-of-the-art assessment, the topic of verification pervades this report. But a word of qualification (and, perhaps, warning) is due, in that "verification" is often employed in a wider sense, and may mean the use of empirical data for anything from calibration of the model to its actual validation. The context must be considered, for a "verified" model may not be all it appears.

3. REPORT CONTENT AND ORGANIZATION

The basic arrangement of this report is to progress from model formulation to solution to specific application. Such a segregation of topics, of course, cannot be strictly observed and there is therefore considerable immixture. Estuarine hydrodynamics, which determine the transport of substances in the estuary, are considered first and organized from the standpoint of spatial dimensionality. Both advective and diffusive processes are discussed. Here, also, the discussion of salinity distribution is undertaken, not only because of the value of salinity as a natural tracer, but because of its considerable influence on estuarine circulation. Then the modeling of water quality parameters per se is treated, which involves the specification of source and sink terms and their incorporation with the transport mechanisms into various conservation relations. The discussion is divided into a treatment of general chemical and biological parameters (Chapter III) and a treatment of temperature (Chapter IV). Temperature is discussed separately for several reasons. It is a parameter which is currently receiving particular attention because of its profound ecological importance. It is a parameter which, like salinity, exhibits significant gradients in estuaries due to the mixing of river and ocean water. Further, because of the dramatic dynamics of thermal discharges, e.g. the large volumes of flow involved and the effects of buoyancy, their modeling requires special consideration.

An appraisal of the use of physical hydraulic models in estuarine quality is presented next (Chapter V) taking advantage thereby of the formulations of mass and momentum transfer developed in the preceding chapters. Solution techniques are discussed in Chapter VI, separated into analog and analog-hybrid techniques, which accomplish the integration of the basic equations continuously (in one independent variable) using electronic components, and numerical methods, in particular finite-difference techniques which involve integration of the equations using finite increments in the independent variables and principally find application with high-speed digital computers. In the latter topic, consideration is given to accuracy and stability problems as well as numerical phenomena such as false diffusion and non-conservation of mass or energy. Several case studies are presented in Chapter VII to provide examples of recent modeling investigations of estuarine water quality. The selection is not intended to be exhaustive but rather to exemplify the present state of model application to estuarine problems. Finally, a brief overview of the estuarine animal populace and present trends in biological modeling in estuaries is given in Chapter VIII. At present, there is very little effort toward incorporating or linking the higher life-forms in estuaries to water quality models, but this is indubitably one of the ultimate directions of estuarine modeling.

In a strict sense, a complete state-of-the-art report on estuarine water quality modeling would encompass a large part of existing knowledge in chemical and biochemical kinetics, the dynamics of nonhomogeneous stratified fluids, boundary and transfer processes at the air-sea interface, modeling of biological and ecological systems, turbulent transport, and so on. For evident reasons, such an ambitious approach was not undertaken here. The emphasis throughout this report is, rather, on the interaction of these phenomena and its formulation. Indeed, the uniquely complex and difficult estuarine system can probably be best characterized by that feature, interaction.

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CHAPTER II

HYDRODYNAMIC MODELS

1. THREE-DIMENSIONAL MODELS

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1.1 INTRODUCTION

In this section the basic time-dependent equations in three spatial dimensions, expressing the conservation of mass, of momentum, and of a dissolved or finely divided suspended constituent of the waters in an estuary, are developed. In order to keep this section from becoming overly long, the development will of necessity be abbreviated, with frequent use of the phrase "it can be shown." However, some outline of the development of the basic equations from first principles is desirable, in order to clearly indicate what terms and processes are neglected in arriving at simplified forms of the equations which offer some possibility of solution, either in terms of our present knowledge or of knowledge which might be gained in the foreseeable future.

This development will include arguments for the neglect of certain terms, particularly certain terms that arise in the averaging process. Again, these arguments must be brief, without extensive observational proof of the statements of relative size of the pertinent terms being considered.

1.1.1 The Coordinate System

Tensor notation will be employed in this section because of the economy it affords in respect to the number of terms which must be written down in expressing the complex differential equations which develop from the first principles to be considered here. Thus, a right-handed rectilinear coordinate system is envisioned with the three axes x_i $(i = 1,2,3)$ oriented such that x_1 and x_2 are in a horizontal plane, and x_3 is the vertical axis directed upwards (i.e., parallel to the force of gravity but positive in the direction of $-\vec{g}$). The plane of $x_3 = 0$ is considered to coincide with mean sea level.

1.1.2 The Concept of the Ensemble Average: Deterministic vs. Stochastic Modes of Motion

The basic conservation principles will first be expressed in terms of the instantaneous field of motion and of the distribution of the pertinent properties of the water in the estuary such as density, salinity and pressure. It has long been recognized that for the real, turbulent conditions of a natural waterway these equations are intractable. Some type of averaging is required in order to separate what might be called the deterministic modes of motion from that part of the motion which is by nature stochastic in character. The method of averaging has considerable influence on the meaning of the individual terms of the resulting equations.

The type of averaging to be initially employed here is based on the following conceptual argument. Assume that the instantaneous fields of motion and of the pertinent properties could be observed, in detail, within an estuary over some time period. During this time period the external processes, i.e., tidal variation at the mouth of the estuary, freshwater inflow, radiation balance and meteorological conditions, are defined--that is, are known functions of time. Now assume that the instantaneous fields of motion and of the pertinent properties in this same estuary were observed over another time period of the same length as the first during which the time variations of the external processes were the same as in the first period, and that the time histories of all the external processes prior to this second period were the same as those prior to the first period, back as far in time as is required by the inherent dynamic "memory" of the system.

If such measurements were possible, it would be found that the fields of motion and of the distribution of pertinent properties would differ in detail from one period to the other, despite the equality of the time variations of the external processes. If k such "identical" periods occurred, the instantaneous field of motion and of the distribution of pertinent properties for any one period would differ, in detail, from all the others.

A part of the instantaneous field of motion would be common to all such k "identical" periods, and this part is called the deterministic mode of motion. A part of the instantaneous field of motion, representing the difference between the instantaneous field of motion for any one of the k "identical" periods and the deterministic mode, constitutes the stochastic mode of motion. These "turbulent" departures in the instantaneous velocity field, at any point in space and at any time relative to the start of each of the k "identical" periods, are distributed among the k periods in accordance with some probability distribution--that is, they are "random" in character, though not necessarily "gaussian". A similar deterministic mode and stochastic mode would exist for each of the instantaneous distributions of the pertinent properties such as density, salinity and pressure.

Note that each of these conceptual k "identical" periods starts at the same point in the identical time histories of the external processes; for example, at the same tidal epoch. If, at a given point in space, the time records of the velocity for each of the k periods were lined up relative to this starting time, and the average at a given point in time were taken across all k records, then the resulting average is called the ensemble average. Such an ensemble average is time dependent, since it is taken at every point in time over all the k periods. A similar operation would provide ensemble averages for the pertinent parameters such as density, salinity and pressure. If k is sufficiently large, the ensemble averages may be taken as suitable approximations to the deterministic modes of motion and of the distribution of the pertinent properties.

It has been more common practice to obtain averages of the instantaneous equations by taking such averages over a time period ΔT small compared to the time scale at which one wishes to resolve the field of motion or the distribution of properties. The problem with this approach is that the stochastic or turbulent mode of motion encompasses a wide range of time and spatial scales.

The ensemble average has the advantage of smoothing out the stochastic mode of motion at all time scales, while also retaining the variations in the deterministic mode at all time scales. Furthermore, this is the average used in most theories of turbulence. The fact that it is only conceptually attainable is not a disadvantage. The predicting equations which can be developed will in any case provide an estimate of the most probable field of motion and/or of properties in the estuary, and not the actual instantaneous velocities and instantaneous values of the pertinent properties which would occur at a real instant of time.

1.1.3 The Notation

The instantaneous velocity at a point x_i and a time t during one of the k "identical" periods is designated by $\tilde{u}_i$. We then define

$$\tilde{u}_i = u_i + u_i' \tag{2.1}$$

and

$$u_i = \langle \tilde{u}_i \rangle_k \tag{2.2}$$

where u_i is the ensemble average of $\tilde{u}_i$ over all k "identical" periods, and u_i' is the departure of the instantaneous velocity for any one of the k periods from the ensemble average. Note that $\langle\ \rangle_k$ represents the operation of obtaining the ensemble average. Further note that

$$\langle u_i' \rangle_k = 0 \tag{2.3}$$

Similar definitions apply to any of the pertinent properties which enter the equations. Thus, in summary:

x_i = a point in space, in the x_1, x_2, x_3 coordinate system.

t = time.

$\tilde{u}_i$ = the instantaneous velocity at a point x_i, and time t during any one of k "identical" periods. $\tilde{u}_1$, $\tilde{u}_2$ and $\tilde{u}_3$ are the rectilinear components, along x_1, x_2 and x_3 respectively, of the velocity $\tilde{u}_i$.

$\tilde{s}$ = the instantaneous concentration (in mass per unit volume) of dissolved salt, at a point x_i and a time t during any one of k "identical" periods.

$\tilde{\rho}$ = the instantaneous density at a point x_i and a time t during any one of k "identical" periods.

$\tilde{p}$ = the instantaneous pressure at a point x_i and a time t during any one of k "identical" periods.

$\tilde{\zeta}$ = the instantaneous concentration of some dissolved or finely suspended constituent at a point x_i and a time t during any one of k "identical" periods.

u_i = the ensemble average of $\tilde{u}_i$ over all k.

s = the ensemble average of $\tilde{s}$ over all k

ρ = the ensemble average of $\tilde{\rho}$ over all k .

p = the ensemble average of $\tilde{p}$ over all k .

ζ = the ensemble average of $\tilde{\zeta}$ over all k .

$(\ )_k$ = symbol for the ensemble averaging operation.

u_i' = the "turbulent" departure of the instantaneous velocity from its ensemble average.

s' = the "turbulent" departure of the instantaneous salt concentration from its ensemble average.

ρ' = the "turbulent" departure of the instantaneous density from its ensemble average.

p' = the "turbulent" departure of the instantaneous pressure from its ensemble average.

ζ' = the "turbulent" departure of the instantaneous concentration of a constituent from its ensemble average.

1.2 THE BASIC EQUATIONS

1.2.1 Conservation of Mass

The basic statement of the principle of conservation of mass is simply that the mass of a moving fluid particle, that is, a particle of fluid whose boundaries move with the instantaneous velocity, remains constant. Thus

$$\frac{d\tilde{M}}{dt} = 0$$

where $\tilde{M}$ is the mass of the moving fluid particle. This statement leads to the differential equation

$$\frac{\partial\tilde{\rho}}{\partial t} + \frac{\partial}{\partial x_i}(\tilde{u}_i\,\tilde{\rho}) = 0 \qquad (2.4)$$

As discussed in Sections 1.1.2 and 1.1.3 above, the ensemble average of this equation is taken, after substituting

$$\tilde{u}_i = u_i + u_i'$$

$$\tilde{\rho} = \rho + \rho'$$

resulting in

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i} (u_i \rho) + \frac{\partial}{\partial x_i} \langle u_i' \rho' \rangle_k = 0 \tag{2.5}$$

Note that while the ensemble means of u_i' and ρ' are zero, the ensemble mean of the cross-product $u_i' \rho'$ is not necessarily zero. However, note that in this case

$$\langle u_i' \rho' \rangle_k = \gamma_{u',\rho'} \left(\langle u_i'^2 \rangle_k \langle \rho'^2 \rangle_k \right)^{\frac{1}{2}}$$

where $\gamma_{u',\rho'}$ designates the correlation coefficient between u_i' and ρ'. The maximum value the correlation coefficient can have is 1.0. The root-mean-square velocity deviation is on the order of 10^{-1} of the ensemble average, and the root-mean-square density deviation is at most on the order of 10^{-3} of the ensemble average density. Consequently

$$\frac{\langle u_i' \rho' \rangle_k}{u_i \rho} \lesssim 10^{-4}$$

and the last term of Equation (2.5) can therefore be neglected, giving finally

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i} (u_i \rho) = 0 \tag{2.6}$$

(Note that this argument is essentially the same as the Boussinesq approximation.)

Making use of the equality

$$\frac{d\rho}{dt} \equiv \frac{\partial \rho}{\partial t} + u_i \frac{\partial \rho}{\partial x_i}$$

Equation (2.6) can also be written as

$$\frac{1}{\rho} \frac{d\rho}{dt} + \frac{\partial u_i}{\partial x_i} = 0 \tag{2.7}$$

It is usually stated that, for an incompressible fluid, $\frac{d\rho}{dt} = 0$ and hence, since the compressibility of water is very small, the equation of continuity applicable to an estuary can be closely approximated by

$$\frac{\partial u_i}{\partial x_i} = 0 \tag{2.8}$$

that is, the three-dimensional flow field must be non-divergent. This equation might be more appropriately called the equation of volume continuity. However, more than simply incompressibility must be invoked to obtain (2.8) from (2.7). The density of estuarine water is a function of temperature, salinity and pressure. Thus

$$\frac{d\rho}{dt} = \left(\frac{\partial\rho}{\partial p}\right)\frac{dp}{dt} + \left(\frac{\partial\rho}{\partial s}\right)\frac{ds}{dt} + \left(\frac{\partial\rho}{\partial\theta}\right)\frac{d\theta}{dt}$$

The statement that a fluid is incompressible means that $\left(\frac{\partial\rho}{\partial p}\right) = 0$. However, this statement does not mean that $\left(\frac{\partial\rho}{\partial s}\right)$ and $\left(\frac{\partial\rho}{\partial\theta}\right)$ are zero. To obtain Equation (2.8) from Equation (2.7) it is necessary to invoke a Boussinesq-type approximation; that is, that time and spatial variations in density may be neglected except in terms in which they are multiplied by gravity. In any case, Equation (2.8) is in fact a good approximation to the equation of continuity for use in estuaries.

1.2.2 Conservation of Momentum

Newton's Second Law is the basic statement of the principle of conservation of momentum; that is, the time rate of change of momentum of a moving elemental fluid particle is equal to the sum of the forces acting on the particle. The differential equation expressing this principle is called the equation of motion. For estuaries the instantaneous equation of motion is given by

$$\frac{\partial}{\partial t}(\tilde{\rho}\,\tilde{u}_i) + \frac{\partial}{\partial x_j}(\tilde{\rho}\,\tilde{u}_i\,\tilde{u}_j) = -\frac{\partial\tilde{p}}{\partial x_i} - 2\varepsilon_{ij\ell}\,\Omega_j\,\tilde{\rho}\,\tilde{u}_\ell + \tilde{\rho}\,g_i + \tilde{\rho}\mu\,\frac{\partial^2\tilde{u}_i}{\partial x_j^2} \qquad (2.9)$$

where $\varepsilon_{ij\ell}$ is the cyclic tensor, g_i the acceleration of gravity, μ the kinematic molecular viscosity, and Ω_j the component of the angular velocity of the earth in the x_j direction.

Now, substituting for the instantaneous value of each of the variables the sum of the ensemble average value and a deviation term, that is

$$\tilde{u}_i = u_i + u_i'$$
$$\tilde{\rho} = \rho + \rho'$$
$$\tilde{p} = p + p'$$

then the x_1, x_2 and x_3 components of the ensemble-averaged equation of motion are

$$\frac{\partial u_1}{\partial t} + \frac{\partial(u_1u_j)}{\partial x_j} = -\frac{1}{\rho}\frac{\partial p}{\partial x_1} + fu_2 + \mu\frac{\partial^2 u_1}{\partial x_j^2} - \frac{\partial}{\partial x_j}\langle u_1'\,u_j'\rangle_k \qquad (2.10)$$

$$\frac{\partial u_2}{\partial t} + \frac{\partial(u_2u_j)}{\partial x_j} = -\frac{1}{\rho}\frac{\partial p}{\partial x_2} - fu_1 + \mu\frac{\partial^2 u_2}{\partial x_j^2} - \frac{\partial}{\partial x_j}\langle u_2'\,u_j'\rangle_k \qquad (2.11)$$

and

$$0 = -\frac{1}{\rho}\frac{\partial p}{\partial x_3} - g \qquad (2.12)$$

where $f = 2\Omega_3 = 2\Omega \sin \varphi$ is the coriolis parameter. Here Ω is the angular velocity of the earth and φ is the latitude.

Some terms have already been neglected in writing these equations in the format shown. First note that in these equations the turbulent pressure fluctuation p' does not appear since in Equation (2.9) the pressure does not appear in a cross-product with any other instantaneous variable. That is,

$$\langle \frac{\partial \tilde{p}}{\partial x_i} \rangle_k = \frac{\partial}{\partial x_i} \langle \tilde{p} \rangle_k = \frac{\partial}{\partial x_i} [\langle p \rangle_k + \langle p' \rangle_k] = \frac{\partial p}{\partial x_i}$$

The first and second step in the above equality result from application of Taylor's Rules regarding ensemble averages. The final step results from the fact that the ensemble average of the ensemble average is the ensemble average (that is, $\langle p \rangle_k = p$) and from $\langle p' \rangle_k = 0$.

Next, note that ρ' does not appear in the above equations because the Boussinesq approximation has been applied. The coriolis terms involving the ensemble average vertical velocity u_3 have been neglected in the two horizontal component equations. Finally, all acceleration terms, both local and inertial, are neglected compared to gravity in the vertical component. Thus the vertical component equation (2.12) is reduced to the hydrostatic equation. Note that by virtue of the equation of continuity, Equation (2.8), the field acceleration term (the second term) in each of the horizontal components of the equation of motion can be written

$$\frac{\partial (u_1 u_j)}{\partial x_j} = u_j \frac{\partial u_1}{\partial x_j}$$

in Equation (2.10), and

$$\frac{\partial (u_2 u_j)}{\partial x_j} = u_j \frac{\partial u_2}{\partial x_j}$$

in Equation (2.11).

Consider now the pressure force term in Equation (2.10). We proceed by integrating the hydrostatic equation, Equation (2.12), from the depth x_3 , where the pressure equals p , to the water surface, $x_3 = \eta$, where the pressure equals p_a , the atmospheric pressure. That is,

$$\int_{x_3}^{\eta} \frac{\partial p}{\partial x_3} dx_3' = -g \int_{x_3}^{\eta} \rho dx_3'$$

or

$$p_a - p = -g \int_{x_3}^{\eta} \rho dx_3'$$

Hence

$$\frac{\partial p}{\partial x_1} = \frac{\partial p_a}{\partial x_1} + g \frac{\partial}{\partial x_1} \int_{x_3}^{\eta} \rho dx_3' \qquad (2.13)$$

Applying Leibnitz' Rule to the last term of (2.13) gives

$$\frac{\partial p}{\partial x_1} = \frac{\partial p_a}{\partial x_1} + g(\rho)_\eta \frac{\partial \eta}{\partial x_1} + g \int_{x_3}^{\eta} \frac{\partial \rho}{\partial x_1} dx_3' \tag{2.14}$$

To the same approximation as the Boussinesq approximation, we may replace $(\rho)_\eta$, the density at the surface, by ρ, the density at depth z, in the second term on the right side of (2.14). Hence

$$\frac{1}{\rho}\frac{\partial p}{\partial x_1} = \frac{1}{\rho}\frac{\partial p_a}{\partial x_1} + g \frac{\partial \eta}{\partial x_1} + \frac{g}{\rho} \int_{x_3}^{\eta} \frac{\partial \rho}{\partial x_1} dx_3' \tag{2.15}$$

Designating the x_1-component of the slope of the pressure surface at depth x_3 relative to the slope of the water surface by $i_{1,p,\eta}$, then

$$\frac{1}{\rho}\frac{\partial p}{\partial x_1} = \frac{1}{\rho}\frac{\partial p_a}{\partial x_1} + g \frac{\partial \eta}{\partial x_1} + g\, i_{1,p,\eta} \tag{2.16}$$

The x_1-component of the ensemble-averaged equation of motion can then be written

$$\frac{\partial u_1}{\partial t} + \frac{\partial (u_1 u_j)}{\partial x_j} = -g \frac{\partial \eta}{\partial x_1} - g\, i_{1,p,\eta} - \frac{1}{\rho}\frac{\partial p_a}{\partial x_1} + f u_2 + \mu \frac{\partial^2 u_1}{\partial x_j^2} - \frac{\partial}{\partial x_j} \langle u_1' u_j' \rangle_k \tag{2.17}$$

Likewise, the x_2-component of the ensemble-averaged equation of motion becomes

$$\frac{\partial u_2}{\partial t} + \frac{\partial (u_2 u_j)}{\partial x_j} = -g \frac{\partial \eta}{\partial x_2} - g\, i_{2,p,\eta} - \frac{1}{\rho}\frac{\partial p_a}{\partial x_2} - f u_1 + \mu \frac{\partial^2 u_2}{\partial x_j^2} - \frac{\partial}{\partial x_j} \langle u_2' u_j' \rangle_k \tag{2.18}$$

where the pressure force term $\frac{1}{\rho}\frac{\partial p}{\partial x_2}$ has been replaced by

$$\frac{1}{\rho}\frac{\partial p}{\partial x_2} = \frac{1}{\rho}\frac{\partial p_a}{\partial x_2} + g \frac{\partial \eta}{\partial x_2} + g\, i_{2,p,\eta} \tag{2.19}$$

The relative isobaric slope terms $i_{1,p,\eta}$ and $i_{2,p,\eta}$ are given by

$$i_{1,p,\eta} = \frac{1}{\rho} \int_{x_3}^{\eta} \frac{\partial \rho}{\partial x_1} dx_3'$$

and (2.20)

$$i_{2,p,\eta} = \frac{1}{\rho} \int_{x_3}^{\eta} \frac{\partial \rho}{\partial x_2} dx_3'$$

The density depends on temperature, salinity and pressure. In the estuary, the pressure dependence is unimportant. The density dependence on temperature and salinity is conveniently expressed in tables issued by the U. S. Navy Oceanographic Office (1966), in terms of the oceanographic function sigma-t; i.e.

$$\sigma_t = 10^3\ (\rho - 1)$$

for ρ expressed in units of the c.g.s. system. Hence

$$\frac{\partial \rho}{\partial x_1} = 10^{-3}\ \frac{\partial \sigma_t}{\partial x_1}$$

and

$$\frac{\partial \rho}{\partial x_2} = 10^{-3}\ \frac{\partial \sigma_t}{\partial x_2}$$

Hence, the relative isobaric slope may be expressed as

$$i_{1,p,\eta} = \frac{10^{-3}}{1+10^{-3}\sigma_t} \int_{x_3}^{\eta} \frac{\partial \sigma_t}{\partial x_1}\, dx_3{}' \qquad (2.21)$$

and

$$i_{2,p,\eta} = \frac{10^{-3}}{1+10^{-3}\sigma_t} \int_{x_3}^{\eta} \frac{\partial \sigma_t}{\partial x_2}\, dx_3{}' \qquad (2.22)$$

Given the spatial distribution of temperature and salinity, then the spatial distribution of σ_t can be obtained from tabular compilations such as USNOO (1966) or from appropriate numerical relationships which have been developed for use in high-speed computers. Equations (2.21) and (2.22) can then be used to compute the relative isobaric slopes $i_{1,p,\eta}$ and $i_{2,p,\eta}$ for use in the horizontal components of the equation of motion.

The slope terms $i_{1,p,\eta}$ and $i_{2,p,\eta}$ arise because the vertical distance between any two isobaric surfaces varies inversely as the mean density in the water layer between these surfaces. These terms, which remain in modified form even in the vertically averaged, two-dimensional equations and the sectionally averaged, one-dimensional equation, have been neglected in numerical models which have been developed to date. In a strong, moderately mixed coastal plane estuary, typical of those which occur along the Atlantic coast of the United States, these terms are not negligible. Consider for example the James River estuary. The mean density of the vertical water column at the mouth of the estuary is approximately 1.025 gm cm^{-3}, while 30 miles up the estuary the mean density is approximately 1.000 gm cm^{-3}. The vertical distance between the water surface and the 10 decibar pressure surface (which occurs at a depth of approximately 10 meters) is therefore about 25 cm (0.82 ft) greater at the upstream location than at the mouth. The mean longitudinal slope of the 10 decibar surface relative to the water surface over this 30 mile distance is therefore 5.5×10^{-6}. Variations in this slope with time over a tidal cycle are relatively small. In this same stretch of the estuary, the longitudinal slope of the water surface $\frac{\partial \eta}{\partial x_1}$ varies with tidal phase from zero to maximum values of about $\pm 1.5 \times 10^{-6}$.

These relative slopes of the pressure surfaces resulting from horizontal variations in density, which are significant in estuaries having relatively strong horizontal salinity gradients, are the primary cause for the characteristic vertical shear in the horizontal current. In such estuaries the seaward-directed flow during the ebb period typically decreases with depth, while the flow directed up the estuary during the flood period typically increases with depth. Consequently there is a net non-tidal circulation with seaward-directed flow in the upper layers of the estuary and a flow directed up the estuary in the lower layers. The intensity of this vertical shear in the current pattern is not necessarily related to the vertical gradient in salinity, as has been pointed out by Hansen and Rattray (1966). That is, vertical mixing may be strong enough in some estuaries to produce near vertical homogeneity in salinity, but the horizontal gradients in salinity, and hence density, may still be sufficient to produce significant vertical shear in the current. Such a vertical shear can be very important in producing longitudinal dispersion of an introduced pollutant.

While, in this treatment, the vertical component of the equation of motion has been reduced to the hydrostatic equation, the vertical velocity remains in certain terms in the horizontal components of the equation; i.e., in the field acceleration terms and in the Reynolds stress terms. Thus it is certainly not a priori evident that the terms $u_3 \, \partial u_1/\partial x_3$, and $\partial \langle u_1' \, u_3' \rangle_k / \partial x_3$ are negligibly small.

In order to put Equations (2.17) and (2.18) into a form which offers any hope of solution, it is necessary to relate the Reynolds stress terms $\langle u_1' \, u_j' \rangle_k$ and $\langle u_2' \, u_j' \rangle_k$ to the ensemble average field of motion. Except at the boundaries, the viscous frictional term is generally small compared to the terms involving the Reynolds stresses. Classically, it has been assumed that the Reynolds stress terms could be replaced by the product of a turbulent or eddy viscosity and the appropriate component of the deformation tensor. That is,

$$\langle u_1' \, u_j' \rangle_k = - \nu_{1,\ell} \left(\frac{\partial u_1}{\partial x_j} + \frac{\partial u_j}{\partial x_1} \right) \tag{2.23}$$

and

$$\langle u_2' \, u_j' \rangle_k = - \nu_{2,\ell} \left(\frac{\partial u_2}{\partial x_j} + \frac{\partial u_j}{\partial x_2} \right) \tag{2.24}$$

where the eddy viscosity $\nu_{1,\ell} = \nu_{1,j}$ when $\ell = j$ and is otherwise zero. Similarly $\nu_{2,\ell} = \nu_{2,j}$ for $\ell = j$ and is otherwise zero. Equations (2.17) and (2.18) may then be written

$$\begin{aligned} \frac{\partial u_1}{\partial t} + \frac{\partial u_1 u_j}{\partial x_j} = {} & -g \frac{\partial \eta}{\partial x_1} - g \, i_{1,p,\eta} - \frac{1}{\rho} \frac{\partial p_a}{\partial x_1} + f u_2 + \frac{\partial}{\partial x_1} \left\{ 2 \nu_{1,1} \frac{\partial u_1}{\partial x_1} \right\} \\ & + \frac{\partial}{\partial x_2} \left\{ \nu_{1,2} \left(\frac{\partial u_1}{\partial x_2} + \frac{\partial u_2}{\partial x_1} \right) \right\} + \frac{\partial}{\partial x_3} \left\{ \nu_{1,3} \left(\frac{\partial u_1}{\partial x_3} + \frac{\partial u_3}{\partial x_1} \right) \right\} \end{aligned} \tag{2.25}$$

and

$$\begin{aligned} \frac{\partial u_2}{\partial t} + \frac{\partial (u_2 u_j)}{\partial x_j} = {} & -g \frac{\partial \eta}{\partial x} - g \, i_{2,p,\eta} - \frac{1}{\rho} \frac{\partial p_a}{\partial x_2} - f u_1 + \frac{\partial}{\partial x_1} \left\{ \nu_{2,1} \left(\frac{\partial u_2}{\partial x_1} + \frac{\partial u_1}{\partial x_2} \right) \right\} \\ & + \frac{\partial}{\partial x_2} \left\{ 2 \nu_{2,2} \frac{\partial u_2}{\partial x_2} \right\} + \frac{\partial}{\partial x_3} \left\{ \nu_{2,3} \left(\frac{\partial u_2}{\partial x_3} + \frac{\partial u_3}{\partial x_2} \right) \right\} \end{aligned} \tag{2.26}$$

These equations have sometimes been further simplified by: (a) assuming $\nu_{1,1} = \nu_{1,2} = \nu_{2,1} = \nu_{2,2} = \nu_H$, the horizontal "Austausch", or horizontal eddy viscosity; (b) assuming $\nu_{1,3} = \nu_{2,3} = \nu_3$, the vertical eddy viscosity; and (c) neglecting $\partial u_1/\partial x_3$ and $\partial u_3/\partial x_2$ in comparison with $\partial u_2/\partial x_3$. The horizontal components of the ensemble mean equation of motion then become

$$\begin{aligned}\frac{\partial u_1}{\partial t} + \frac{\partial (u_1 u_j)}{\partial x_j} = -g \left(\frac{\partial \eta}{\partial x_1} + i_{1,p,\eta}\right) - \frac{1}{\rho}\frac{\partial p_a}{\partial x_1} + fu_2 + \frac{\partial}{\partial x_1}\left\{2\nu_H \frac{\partial u_1}{\partial x_1}\right\} \\ + \frac{\partial}{\partial x_2}\left\{\nu_H \left(\frac{\partial u_1}{\partial x_2} + \frac{\partial u_2}{\partial x_1}\right)\right\} + \frac{\partial}{\partial x_3}\left\{\nu_3 \frac{\partial u_1}{\partial x_3}\right\}\end{aligned} \tag{2.27}$$

and

$$\begin{aligned}\frac{\partial u_2}{\partial t} + \frac{\partial (u_2 u_j)}{\partial x_j} = -g \left(\frac{\partial \eta}{\partial x_2} + i_{2,p,\eta}\right) - \frac{1}{\rho}\frac{\partial p_a}{\partial x_2} - fu_1 + \frac{\partial}{\partial x_1}\left\{\nu_H \left(\frac{\partial u_2}{\partial x_1} + \frac{\partial u_1}{\partial x_2}\right)\right\} \\ + \frac{\partial}{\partial x_2}\left\{2\nu_H \frac{\partial u_2}{\partial x_2}\right\} + \frac{\partial}{\partial x_3}\left\{\nu_3 \frac{\partial u_2}{\partial x_3}\right\}\end{aligned} \tag{2.28}$$

There does not exist any clear direct observational or theoretical evidence for further simplifying these equations, even though some indirect evidence will be used later in this section in further modifying them. It should also be noted that the coefficients of eddy viscosity are functions of position and, perhaps, time. They are dependent upon the intensity of the turbulent velocity fluctuations, and hence probably on the velocity, the boundary roughness and distance from the boundary, but the relationships are not known. The vertical eddy viscosity must also be dependent upon the vertical stability, or more probably the Richardson Number.

In any case, Equations (2.27) and (2.28), together with Equations (2.21) and (2.22) and the equation of continuity (2.8), are the equations which one must start with in developing a three-dimensional dynamic model of an estuary. If the goal is to develop a dynamic model capable of computing the time dependent surface elevation η and the three components of the time-dependent velocity u_i , these equations, standing alone, in the form given, are insoluble, since there are more unknowns than equations. However, there are several possible procedures for overcoming the difficulty.

In Section 2 of this chapter a two-dimensional vertical-averaged model is developed. In that model the surface elevation η appears as a dependent variable. Assuming for the moment that such a two-dimensional model can be shown to provide satisfactory estimates of the time and space variations in η , even for estuaries with significant vertical and horizontal variations in salinity (and hence density) and with vertical shear in the velocity field, then such a two-dimensional model could be used to determine η , as well as the vertical mean values of the two horizontal velocity components. Thus, given η as a function of time and position, Equations (2.8), (2.27), and (2.28), together with the auxiliary equations (2.21) and (2.22) for determining the relative slope terms, could theoretically be solved, by appropriate numerical means, to obtain the time-dependent three-dimensional velocity field.

In order to make such an approach possible, however, it will be necessary to develop empirical and/or theoretical relationships for the coefficients of eddy viscosity in terms of known or computable parameters.

It should also be pointed out that the slope terms $i_{1,p,\eta}$ and $i_{2,p,\eta}$ depend upon the spatial distribution of density and hence of salinity. Consequently the dynamic model cannot be used to compute the field of motion, which then would be used in the determination of the distribution of salinity. The equations of salt continuity, to be developed in the next sub-section, must be solved simultaneously with the dynamic equations.

1.2.3 Conservation of Dissolved Constituents

The differential equation expressing the conservation of salt, in three-dimensions, for instantaneous values of the salt concentration and the velocity, may be written

$$\frac{\partial \tilde{s}}{\partial t} = - \frac{\partial}{\partial x_i} (\tilde{u}_i \tilde{s}) + D \frac{\partial^2 \tilde{s}}{\partial x_i^2} \qquad (2.29)$$

where D is the molecular diffusivity. Proceeding as in the cases for conservation of mass and of momentum, the ensemble average salt balance equation is given by

$$\frac{\partial s}{\partial t} = - \frac{\partial}{\partial x_i} (u_i s) - \frac{\partial}{\partial x_i} \langle u_i' s' \rangle_k + D \frac{\partial^2 s}{\partial x_i^2} \qquad (2.30)$$

Note that, using the equation of continuity $\partial u_i / \partial x_i = 0$, the first term on the right side of (2.30) may also be written

$$\frac{\partial}{\partial x_i} (u_i s) = u_i \frac{\partial s}{\partial x_i}$$

In order to make Equation (2.30) tractable, it is usual to replace the non-advective flux terms by Fickian-type diffusion terms. That is,

$$\langle u_i' s' \rangle_k = -K_\ell \frac{\partial s}{\partial x_i} \qquad (2.31)$$

where $K_\ell = K_i$ for $\ell = i$ and otherwise is zero. Then Equation (2.31) is written

$$\frac{\partial s}{\partial t} = - \frac{\partial}{\partial x_i} (u_i s) + \frac{\partial}{\partial x_1} \left\{K_H \frac{\partial s}{\partial x_1}\right\} + \frac{\partial}{\partial x_2} \left\{K_H \frac{\partial s}{\partial x_2}\right\} + \frac{\partial}{\partial x_3} \left\{K_3 \frac{\partial s}{\partial x_3}\right\} \qquad (2.32)$$

where the molecular diffusion term has been neglected compared to the eddy diffusion terms, and it has been assumed that $K_1 = K_2 = K_H$, the horizontal eddy diffusivity.

As in the case of the coefficients of eddy viscosity, there does not exist an adequate theoretical or empirical basis for relating the coefficients of eddy diffusivity to the ensemble mean velocity distribution and to the distribution of density.

However, some limited evidence does exist which can be used to at least indicate further simplifications of the three-dimensional conservation equations, and also a possible format for relating the eddy coefficients to known or computable parameters. Before proceeding with such a further treatment, however, consider the general form of the equation expressing the balance for a dissolved constituent other than salinity, for which there may be internal sources and sinks.

In Equation (2.32), it has been assumed that salt is conserved within the water body; that is, that there are no internal sources and sinks for salt. Sources and sinks may exist at the boundaries, however. For example, the vertical diffusion term takes on a boundary value at the water surface equal to the effective flux of salt across the boundary resulting from the difference between evaporation and precipitation. In the case of a dissolved substance which is not conserved within the water body, such as an oxidizable pollutant or a radioactive material subject to decay, additional terms must appear in the equation.

Designating the ensemble-averaged concentration of a non-conservative material by ζ, then the three-dimensional equation expressing the local time rate of change of concentration is given by

$$\frac{\partial \zeta}{\partial t} = - \frac{\partial}{\partial x_i} (u_i \zeta) - \frac{\partial}{\partial x_i} \langle u_i' \zeta' \rangle_k + D \frac{\partial^2 \zeta}{\partial x^2} + r_g - r_d \qquad (2.33)$$

where r_g is the mass rate of generation of substance per unit volume and r_d is the mass rate of decay of substance per unit volume. Again, expressing the non-advective flux $\langle u_i' \zeta' \rangle_k$ in terms of an eddy diffusivity and incorporating the molecular diffusion term into this turbulent diffusion term, Equation (2.33) takes the form

$$\frac{\partial \zeta}{\partial t} = - \frac{\partial}{\partial x_i} (u_i \zeta) + \frac{\partial}{\partial x_1} \left\{ K_H \frac{\partial \zeta}{\partial x_1} \right\} + \frac{\partial}{\partial x_2} \left\{ K_H \frac{\partial \zeta}{\partial x_2} \right\} + \frac{\partial}{\partial x_3} \left\{ K_3 \frac{\partial \zeta}{\partial x_3} \right\} + r_g - r_d \qquad (2.34)$$

1.2.4 Some Possible Further Simplification of the Three-Dimensional Conservation Equations for Mass, Momentum and Salt

Studies of one-dimensional and two-dimensional models of conservation of mass, momentum and salt, and of one-dimensional and two-dimensional water quality models, suggest the following:

(a) The greater the detail provided by the model with respect to variations in velocity in time and space, the less significant are the horizontal eddy diffusion terms, and probably the horizontal eddy viscous terms.

(b) In the vertically averaged two-dimensional equations of motion, the bottom boundary frictional term is satisfactorily represented by a term of the form

$$g \frac{u(u^2 + v^2)^{\frac{1}{2}}}{C_h^2}$$

where C_h is the Chezy coefficient.

(c) In a study of the James River estuary using a tidal mean, lateral-averaged two-dimensional equation of motion, Pritchard (1956) showed that the field acceleration term $\bar{u}_3 \, \partial \bar{u}_1 / \partial x_3$ is small compared to other terms in the equation.

These observations suggest that the three-dimensional equations expressing conservation of mass, momentum, and salt might be further simplified as follows:

(a) In the x_1-component of the equation of motion, Equation (2.27), neglect the field acceleration term $u_3\,\partial u_1/\partial x_3$ and the horizontal eddy viscous terms $\partial/\partial x_1\,\{2\nu_H\,\partial u_1/\partial x_1\}$ and $\partial/\partial x_2\,\{\nu_H(\partial u_1/\partial x_2 + \partial u_2/\partial x_1)\}$

(b) In the x_2-component of the equation of motion, Equation (2.28), neglect the field acceleration term $u_3\,\partial u_2/\partial x_3$, and the horizontal eddy viscous terms $\partial/\partial x_1\,\{\nu_H(\partial u_2/\partial x_1 + \partial u_1/\partial x_2)\}$ and $\partial/\partial x_2\,\{2\nu_H\,\partial u_2/\partial x_2\}$

(c) In the salt balance equation, Equation (2.32), neglect the horizontal eddy diffusion terms $\partial/\partial x_1\,\{K_H\,\partial s/\partial x_1\}$ and $\partial/\partial x_2\,\{K_H\,\partial s/\partial x_2\}$

The x_1-component of the equation of motion then becomes

$$\frac{\partial u_1}{\partial t} + u_1\frac{\partial u_1}{\partial x_1} + u_2\frac{\partial u_1}{\partial x_2} = -g\frac{\partial \eta}{\partial x_1} - g\,i_{1,p,\eta} - \frac{1}{\rho}\frac{\partial p_a}{\partial x_1} + fu_2 + \frac{\partial}{\partial x_3}\left\{\nu_3\frac{\partial u_1}{\partial x_3}\right\} \tag{2.35}$$

the x_2-component of the equation of motion then becomes:

$$\frac{\partial u_2}{\partial t} + u_1\frac{\partial u_2}{\partial x_1} + u_2\frac{\partial u_2}{\partial x_2} = -g\frac{\partial \eta}{\partial x_2} - g\,i_{2,p,\eta} - \frac{1}{\rho}\frac{\partial p_a}{\partial x_2} - fu_1 + \frac{\partial}{\partial x_3}\left\{\nu_3\frac{\partial u_2}{\partial x_3}\right\} \tag{2.36}$$

and the salt balance equation becomes

$$\frac{\partial s}{\partial t} = -\frac{\partial}{\partial x_1}(u_1 s) + \frac{\partial}{\partial x_3}\left\{K_3\frac{\partial s}{\partial x_3}\right\} \tag{2.37}$$

The auxiliary Equations (2.21) and (2.22) must still be used to compute the relative isobaric slopes $i_{1,p,\eta}$ and $i_{2,p,\eta}$ from the horizontal and vertical distribution of density (salinity). Also, the equation of continuity in the form given in Equation (2.8), that is

$$\frac{\partial u_1}{\partial x_1} = 0$$

must be also solved simultaneously with the dynamic equations and the salt balance equation.

The solutions to these equations must satisfy the following vertical integral conditions:

$$\begin{aligned}\int_{-\xi}^{\eta}\left\{\frac{\partial u_1}{\partial t} + u_1\frac{\partial u_1}{\partial x_1} + u_2\frac{\partial u_1}{\partial x_2} + g\,i_{1,p,\eta} - fu_2\right\}dx_3 \\ = -g\,(\xi+\eta)\frac{\partial \eta}{\partial x_1} - \frac{(\xi+\eta)}{\rho_h}\frac{\partial p_a}{\partial x_1} + \tau_{w,1} - g\,\frac{u_{1,h}(u_{1,h}^2 + u_{2,h}^2)^{\frac{1}{2}}}{C_h^2}\end{aligned} \tag{2.38}$$

$$\begin{aligned}\int_{-\xi}^{\eta}\left\{\frac{\partial u_2}{\partial t} + u_1\frac{\partial u_2}{\partial x_1} + u_2\frac{\partial u_2}{\partial x_2} + g\,i_{2,p,\eta} + fu_1\right\}dx_3 \\ = -g\,(\xi+\eta)\frac{\partial \eta}{\partial x_2} - \frac{(\xi+\eta)}{\rho_h}\frac{\partial p_a}{\partial x_2} + \tau_{w,2} - g\,\frac{u_{2,h}(u_{1,h}^2 + u_{2,h}^2)^{\frac{1}{2}}}{C_h^2}\end{aligned} \tag{2.39}$$

$$\frac{\partial}{\partial x_1}\int_{-\xi}^{\eta} u_1\, dx_3 + \frac{\partial}{\partial x_2}\int_{-\xi}^{\eta} u_2\, dx_3 = -\frac{\partial \eta}{\partial t} \tag{2.40}$$

and

$$\frac{\partial}{\partial t}\int_{-\xi}^{\eta} s\, dx_3 + \frac{\partial}{\partial x_1}\int_{-\xi}^{\eta} (u_1 s)\, dx_3 + \frac{\partial}{\partial x_2}\int_{-\xi}^{\eta} (u_2 s)\, dx_e = S_h(E-P) \tag{2.41}$$

where $-\xi$ is the x_3 value at the bottom, $(E-P)$ is the difference between evaporation and precipitation at the water surface, expressed in units of length per unit time, $\tau_{w,1}$ and $\tau_{w,2}$ are the x_1 and x_2 components of the wind stress at the surface, and the subscript h implies a vertical average. That is,

$$u_{1,h} = \frac{1}{(\xi+\eta)}\int_{-\xi}^{\eta} u_1\, dx_3 \tag{2.42}$$

$$u_{2,h} = \frac{1}{(\xi+\eta)}\int_{-\xi}^{\eta} u_2\, dx_3 \tag{2.43}$$

$$s_h = \frac{1}{(\xi+\eta)}\int_{-\xi}^{\eta} s\, dx_3 \tag{2.44}$$

The solutions to the three-dimensional equations must also satisfy the following cross-section integral conditions, where in order to simplify the notation it is assumed that the coordinate system is oriented such that x_1 is directed along the axis of the estuary, and the cross section at any point x_1 has an area σ and is in the plane perpendicular to x_1:

$$\frac{\partial}{\partial x_1}\iint_{\sigma} u_1\, d\sigma = -\frac{\partial \sigma}{\partial t} \tag{2.45}$$

and

$$\frac{\partial}{\partial t}\iint_{\sigma} s\, d\sigma + \frac{\partial}{\partial x_1}\iint_{\sigma} u_1 s\, d\sigma = \frac{(E-P)b_{\eta}}{\sigma}\iint_{\sigma} s\, d\sigma \tag{2.46}$$

For the coastal plane or drowned river valley estuaries characteristic of the Atlantic Coast of the United States, which in their upper reaches extend into the fresh water tidal river, and are bounded at their upper end by the position where the rise and fall of the tide and the tidal oscillations in the current are reduced to zero, an additional integral condition can be obtained. If Equations (2.45) and (2.46) are integrated from $x_1 = (x_1)_o$ where the integrated flow through the cross section equals the river flow Q_R to a cross section in the estuary proper located at x_1, then

$$\iint_{\sigma} u_1\, d\sigma = Q_R - \frac{\partial}{\partial t}\left\{\int_{(x_1)_o}^{x_1} \sigma\, dx_1\right\} \tag{2.47}$$

and

$$\iint_{\sigma} u_1 s\, d\sigma = \int_{(x_1)_o}^{x_1}\left\{\frac{(E-P)b_{\eta}}{\sigma}\iint_{\sigma} s\, d\sigma\right\} dx_1 - \frac{\partial}{\partial t}\left[\int_{(x_1)_o}^{x_1}\left\{\iint_{\sigma} s\, d\sigma\right\} dx_1\right] \tag{2.48}$$

Equations (2.8), (2.35), (2.36) and (2.37), expressing the conservation of mass, momentum and salt in three spatial dimensions, plus Equations (2.38), (2.39), (2.40), (2.41), (2.45), (2.46), (2.47) and (2.48) expressing the integral boundary conditions, together with the auxiliary Equations (2.21) and (2.22), represent a set of equations which, on the basis of present knowledge, include the most important processes controlling the dynamics and kinematics of an estuary. As such, these equations offer a suitable basis for a three-dimensional, numerical model of an estuary.

The dependent variables to be computed from such a model are: (a) the surface elevation of the estuary η as a function of horizontal position (x_1, x_2) and of time t ; (b) the three velocity components, u_1, u_2 and u_3, as a function of horizontal position and depth (x_1, x_2, x_3) and of time t ; and (c) the salinity s as a function of horizontal position and depth (x_1, x_2, x_3) and of time t. The necessary inputs to the model are: (a) the physical dimensions of the estuary, i.e., the horizontal boundaries and the distribution of depth at, say, mean low water; (b) the temporal and spatial distribution of atmospheric pressure and of surface wind stress over the period covered by the computation; (c) values of the vertical coefficients of eddy viscosity ν_3 and eddy diffusivity K_3 as a function of position (x_1, x_2, x_3) and time during the period covered by the computations; (d) values of the water density ρ as a function of position (x_1, x_2, x_3) and time during the period covered by the computations; (e) the fresh water inflow to the estuary as a function of time during the period covered by the computations; (f) values of the difference, evaporation minus precipitation, at the water surface of the estuary, as a function of horizontal position (x_1, x_2) and time during the period covered by the computations; (g) the elevation of the water surface η along the line marking the seaward boundary of the estuary, as a function of time during the period covered by the computations; (h) values of the salinity s in the cross-section marking the seaward boundary of the estuary, as a function of time during the period covered by the computations; and (i) an initial set of values of the dependent variables at all positions in the estuary.

The spatial and temporal distribution of density is required for computations of the relative isobaric slopes $i_{1,p,\eta}$ and $i_{2,p,\eta}$ from Equations (2.21) and (2.22). The density of the estuarine water depends on temperature and salinity. In estuaries in which the relative isobaric slopes contribute significantly to the dynamic balance, salinity variations are generally much more important than temperature variations in determining density variations. Consequently it should be adequate to assume either a constant water temperature throughout the estuary, or a time independent spatial distribution of temperature characteristic of the period covered by the computations. The initial distribution of salinity would then be used, together with the assumed temperature, to determine the initial spatial distribution of density. Equations (2.21) and (2.22) would then be used to compute initial values of the relative isobaric slopes $i_{1,p,\eta}$ and $i_{2,p,\eta}$ as a function of position (x_1, x_2, x_3). After each time step in the computation, the new distribution of salinity would be used with the assumed distribution of temperature to determine the spatial distribution of density, from which new values of $i_{1,p,\eta}$ and $i_{2,p,\eta}$ would be found for use in the next time step.

The major remaining unknown input terms for the proposed model are values of the vertical eddy viscosity ν_3 and the vertical eddy diffusivity K_3. Some evidence is available as to the relationship of K_3 to the geometry of the estuary, the velocity shear and the vertical stability. Presumably the eddy viscosity would depend on these parameters in a similar manner. However, research is required to develop generally applicable relationships such that ν_3 and K_3 can be determined from known and/or computable parameters.

Pritchard (1960) using the results of studies made in the James River (Pritchard 1954, Kent and Pritchard 1959) found that for tidal mean, lateral-averaged data, the vertical eddy diffusivity was related to the mean tidal velocity $|\bar{u}|$, the water depth h, the height H, period T, and wave length L of the surface wind waves, and the Richardson Number R_i by the equation

$$K_3(Z) = \eta|\bar{u}| \frac{Z^2(h-Z)^2}{h^3} (1+\beta R_i)^{-2} + \xi \frac{Z(h-Z)}{h} \frac{H}{T} e^{-2\pi Z/L} (1+\beta R_i)^{-2} \qquad (2.49)$$

where Z is the vertical distance below the water surface (i.e., $Z = \eta - x_3$), h is the vertical distance between the water surface and the bottom, and η, ξ, and β are non-dimensional constants. For the James River estuary, the numerical value of these coefficients were: $\eta = 8.59 \times 10^{-3}$; $\xi = 9.57 \times 10^{-3}$; and $\beta = 0.276$. This equation is based on data collected during one relatively short time interval in one segment of one estuary. It is based on tidal mean data. The degree to which these results can be extended to other estuaries and to conditions of time-varying currents within the tidal cycle is not known.

For an estuary which is vertically homogeneous and for calm wind conditions, Equation (2.49) reduces to

$$K_3(Z) = 9.59 \times 10^{-3} |\bar{u}| \frac{Z^2(h-Z)^2}{h^3} \qquad (2.50)$$

Bowden (1960) computed values of the vertical eddy diffusivity for the Mersey estuary, which was only slightly stratified during the period of study. His results show a vertical variation in K_3 similar to that defined by Equation (2.50). The mid-depth values of K_3 as computed by Bowden for the Mersey estuary were 27 $cm^2\ sec^{-1}$ for one period of observation, and 30 $cm^2\ sec^{-1}$ for another period. At mid-depth, Equation (2.50) reduces to

$$K_3(Z=\tfrac{1}{2}h) = 5.37 \times 10^{-4} |\bar{u}|\, h \qquad (2.51)$$

In the Mersey, $|\bar{u}| \approx 50$ cm sec^{-1}, and the depth at the point of observation was $h \approx 20$ meters. Hence Equation (2.51) gives a value of K_3 at mid-depth of about 54 $cm^2\ sec^{-1}$. Bowden (1960) states that despite the relatively weak vertical stability, it was still sufficient to significantly reduce the vertical eddy diffusivity. Bowden also determined the vertical eddy viscosity for the Mersey estuary. He found ν_3 to vary with depth in very nearly the same manner as K_3, but to have values about twice as large as K_3.

The algorithms necessary to express the differential and integral equations which provide the basis of the proposed model in a format suitable for numerical solution by high-speed computer have not yet been fully developed, though elements of the required system of algorithms do exist. It is likely that such a three-dimensional numerical model of the dynamic and kinematic behavior of a real estuary would require considerable computational time on a very large computer.

2. TWO-DIMENSIONAL MODELS

D. W. Pritchard

2.1 INTRODUCTION

The basic time-dependent equations expressing the conservation of mass, momentum, and of a dissolved constituent of the waters of an estuary, in three spatial dimensions, as developed in Section 1 of this chapter, will serve as the starting point for the treatment of two-dimensional models of an estuary to be presented in this section. This section will include discussions of the significance of terms which are neglected and of simplifying assumptions which are made in order to develop a model composed of a tractable set of equations. Where adequate descriptions are already available in scientific publications or technical reports, existing models will be referred to, but not described in detail.

2.1.1 The Coordinate System and the Notations to be Used

In Section 1 of this chapter tensor notation was employed in conjunction with a right-handed rectilinear coordinate system, x_i , with the x_1 and x_2 axes lying in a horizontal plane coincident with the plane of mean tide level, and the x_3-axis directed upwards, positive in the direction opposite to the acceleration of gravity. In this section it will generally be more convenient to employ an x-y-z rectilinear coordinate system, and a vector-scalar notation system. The x- and y-axes are considered to lie in the horizontal plane coincident with the plane of mean tide level, and the z-axis is directed upwards. Thus the x-axis corresponds to the x_1-axis; the y-axis corresponds to the x_2-axis; and the z-axis corresponds to the x_3-axis. The ensemble average velocity components along the x-, y-, and z-axis will be designated by u, v, and w, respectively. Thus u in the notation to be employed in this section corresponds to u_1 in the notation used in Section 1. Likewise, v corresponds to u_2 , and w to u_3 .

Much of the remaining notation used in Section 1 can be carried over directly to this section. Where confusion might result, special note is made in the text.

2.2 THE BASIC EQUATIONS FOR A VERTICALLY AVERAGED TWO-DIMENSIONAL MODEL

2.2.1 Conservation of Mass

We start with Equation (2.6), the ensemble mean equation of mass continuity in three spatial dimensions as developed in Section 1. In the notation used in this section, that equation is written

$$\frac{\partial \rho}{\partial t} + \frac{\partial (u\rho)}{\partial x} + \frac{\partial (v\rho)}{\partial y} + \frac{\partial (w\rho)}{\partial z} = 0 \tag{2.52}$$

Now consider that, at any point (x,y,z), the value of the density and of each of the velocity components is equal to the sum of the vertical mean value of that variable taken over the water depth plus a deviation term representing the difference between the value of that variable at the point (x, y, z) and the vertical mean value of that variable. That is, we designate

$$\begin{aligned} \rho &= \rho_h + \rho_h' \\ u &= u_h + u_h' \\ v &= v_h + v_h' \\ w &= w_h + w_h' \end{aligned} \tag{2.53}$$

where

$$\begin{aligned} \rho_h &= \frac{1}{(\xi+\eta)} \int_{-\xi}^{\eta} \rho \, dz = \langle \rho \rangle_h \\ u_h &= \frac{1}{(\xi+\eta)} \int_{-\xi}^{\eta} u \, dz = \langle u \rangle_h \\ v_h &= \frac{1}{(\xi+\eta)} \int_{-\xi}^{\eta} v \, dz = \langle v \rangle_h \\ w_h &= \frac{1}{(\xi+\eta)} \int_{-\xi}^{\eta} w \, dz = \langle w \rangle_h \end{aligned} \tag{2.54}$$

Note from above that use has been made of the following notation for the mean value over the total water depth at time t:

$$\langle f \rangle_h \equiv \frac{1}{(\xi+\eta)} \int_{-\xi}^{\eta} f \, dz \tag{2.55}$$

where f is any spatial-dependent variable, η is the surface elevation, $-\xi$ is the z value at the bottom, and $h = (\xi+\eta)$ is the total water depth at the time t. Hence, from (2.53) and (2.54), we note that

$$\langle \rho_h' \rangle_h = \langle u_h' \rangle_h = \langle v_h' \rangle_h = \langle w_h' \rangle_h = 0 \tag{2.56}$$

Substituting from Equation (2.53) into Equation (2.52) and taking the integral of that equation over the total depth $h = (\xi+\eta)$ gives

$$\frac{\partial}{\partial t}(h\rho_h) + \frac{\partial}{\partial x}(hu_h\rho_h) + \frac{\partial}{\partial y}(hv_h\rho_h) + \frac{\partial}{\partial x}(h\langle u_h'\rho_h'\rangle_h) + \frac{\partial}{\partial y}(h\langle v_h'\rho_h'\rangle_h) = 0 \tag{2.57}$$

Note that even though $\langle \rho_h' \rangle_h = \langle u_h' \rangle_h = \langle u_h' \rangle_h = 0$, the cross-product terms $\langle u_h' \rho_h' \rangle_h$ and $\langle v_h' \rho_h' \rangle_h$ are not necessarily zero. However, in this case it is well known that

$$\frac{\langle u_h' \rho_h' \rangle_h}{u_h \rho_h} < 1$$

and

$$\frac{\langle v_h' \rho_h' \rangle_h}{v_h \rho_h} \ll 1$$

i.e., these ratios are on the order of 10^{-4} or less. Thus, the last two terms in (2.57) may be neglected. Expanding the differentials, and using the equality $\partial h/\partial t = \partial \eta/\partial t$ (since $h = \xi + \eta$ and $\partial \xi/\partial t = 0$), Equation (2.57) can be written

$$\frac{h}{\rho_h} \frac{\partial \rho_h}{\partial t} + \frac{\partial (hu_h)}{\partial x} + \frac{\partial (hv_h)}{\partial y} = - \frac{\partial \eta}{\partial t} \tag{2.58}$$

As discussed in Section 1, the first term in (2.58) may be neglected for a fluid such as water which has a very small compressibility, and for which the Boussinesq approximation is appropriate. Consequently, the equation of continuity of mass in two-dimensions is reduced to

$$\frac{\partial (hu_h)}{\partial x} + \frac{\partial (hv_h)}{\partial y} = - \frac{\partial \eta}{\partial t} \tag{2.59}$$

2.2.2 Conservation of Momentum

The three-dimensional ensemble-averaged equations of motion in the form given by Equations (2.17) and (2.18) of Section 1 of this chapter serve as the starting point for the development of a vertically averaged, two-dimensional model of the dynamics of an estuary. In the notation used in this section, these equations are (omitting the molecular viscous term)

$$\frac{\partial u}{\partial t} + \frac{\partial u^2}{\partial x} + \frac{\partial uv}{\partial x} + \frac{\partial uw}{\partial z} = -g \frac{\partial \eta}{\partial x} -g \, i_{x,p,\eta} - \frac{1}{\rho} \frac{\partial p_a}{\partial x} + fv - \frac{\partial}{\partial x} \langle u'^2 \rangle_k - \frac{\partial}{\partial y} \langle u'v' \rangle_k - \frac{\partial}{\partial z} \langle u'w' \rangle_k \tag{2.60}$$

and

$$\frac{\partial v}{\partial t} + \frac{\partial uv}{\partial x} + \frac{\partial v^2}{\partial y} + \frac{\partial vw}{\partial z} = -g \frac{\partial \eta}{\partial y} -g \, i_{y,p,\eta} - \frac{1}{\rho} \frac{\partial p_a}{\partial x} - fu - \frac{\partial}{\partial x} \langle u'v' \rangle_k - \frac{\partial}{\partial y} \langle v'^2 \rangle_k - \frac{\partial}{\partial z} \langle v'w' \rangle_k \tag{2.61}$$

Now, we introduce into these equations

$$u = u_h + u_h'$$

$$v = v_h + v_h'$$

$$w = w_h + w_h'$$

and integrate the equations from the bottom $(z = -\xi)$ to the surface $(z = \eta)$. The resulting equations are

$$\frac{\partial u_h}{\partial t} + u_h \frac{\partial u_h}{\partial x} + v_h \frac{\partial u_h}{\partial y} = -g \left\{\frac{\partial \eta}{\partial x} + \langle i_{x,p,\eta}\rangle_h\right\} - \frac{1}{\rho_h} \frac{\partial p_a}{\partial x} + f v_h - \frac{1}{h} \frac{\partial}{\partial x} \left\{h\langle {u_h}'^2 + \langle u'^2\rangle_k\rangle_h\right\}$$

$$- \frac{1}{h} \frac{\partial}{\partial y} \left\{h\langle {u_h}'{v_h}' + \langle u'v'\rangle_k\rangle_h\right\} + \frac{1}{h\rho_h} \tau_{w,x} - \frac{1}{h\rho_h} \tau_{B,x} \tag{2.62}$$

and

$$\frac{\partial v_h}{\partial t} + u_h \frac{\partial v_h}{\partial x} + v_h \frac{\partial v_h}{\partial y} = -g \left\{\frac{\partial \eta}{\partial y} + \langle i_{y,p,\eta}\rangle_h\right\} - \frac{1}{\rho_h} \frac{\partial p_a}{\partial y} - f u_h - \frac{1}{h} \frac{\partial}{\partial x} \left\{h\langle {u_h}'{v_h}' + \langle u'v'\rangle_k\rangle_h\right\}$$

$$- \frac{1}{h} \frac{\partial}{\partial y} \left\{h\langle {v_h}'^2 + \langle v'^2\rangle_k\rangle_h\right\} + \frac{1}{h\rho_h} \tau_{w,y} - \frac{1}{h\rho_h} \tau_{B,x} \tag{2.63}$$

where $\tau_{w,x}$ and $\tau_{w,y}$ are the x- and y-components of the surface wind stress, while $\tau_{B,x}$ and $\tau_{B,y}$ are the x- and y-components of the bottom stress. This last term in each equation has usually been replaced by a term of the form

$$\frac{1}{h\rho_h} \tau_{B,x} = g \frac{u_h({u_h}^2 + {v_h}^2)^{\frac{1}{2}}}{h\, {C_h}^2} \tag{2.64}$$

and

$$\frac{1}{h\rho_h} \tau_{B,y} = g \frac{v_h({u_h}^2 + {v_h}^2)^{\frac{1}{2}}}{h\, {C_h}^2} \tag{2.65}$$

where C_h is the Chezy coefficient.

These forms of the equation of motion are similar to the equations used by Leendertse (1967) and by Masch et al. (1969), among others, in formulating a two-dimensional dynamic model of an estuary, but with two rather significant differences.

Equations (2.62) and (2.63) each include a term which arises from the relative slope of the pressure surfaces due to the horizontal variation in density (salinity). The term $\langle i_{x,p,\eta}\rangle_h$ is the y-component of this same slope. The significance of this term in the drowned river valley estuaries of the Atlantic Coast was discussed for the case of the three-dimensional equation in Section 1 of this chapter. At this time we might note that in the James River estuary, for example, the vertical-averaged value of the longitudinal component of the relative isobaric slope has been observed to be about 2.7×10^{-6}, and relatively independent of time over a tidal cycle. This amounts to about 36% of the mean magnitude of the slope of the water surface, averaged over a tidal cycle. That is, in this estuary the longitudinal slope of the water surface $\partial\eta/\partial x$ varies with tidal phase from zero to maximum values of about $\pm 1.5 \times 10^{-5}$.

Each of these equations also contains terms of the type $\langle {u_h}'^2 + \langle u'^2\rangle_k\rangle_h$ and $\langle {u_h}'{v_h}' + \langle u'v'\rangle_k\rangle_h$. The parts of these terms representing ensemble averages of the turbulent velocity fluctuations, $\langle v'^2\rangle_h$, $\langle {u_h}'^2\rangle_h$ and $\langle {u_h}'{v_h}'\rangle_h$, represent the vertical averages of the cross-products of the velocity departures at any depth from the vertical average velocity.

If the velocity field has a vertical shear which is predominantly of one sign, then these terms can be of significant size. In the typical drowned river valley estuary, the vertical shear of the horizontal velocity is predominantly of one sign; i.e., if x is oriented along the axis of the estuary toward the sea, then $\partial u/\partial z$ is predominantly positive.

It can be argued that terms of the type $\langle u_h' v_h' \rangle_h$ can be replaced by the product of a coefficient, having the dimensions of kinematic viscosity, times an appropriate component of the deformation tensor, as was done with the ensemble average terms such as $\langle u'v' \rangle_k$. That is, we might assume that

$$\langle u_h'^2 + \langle u'^2 \rangle_k \rangle_h = -2\nu_{x,x} \frac{\partial u_h}{\partial x}$$

$$\langle u_h' v_h' + \langle u'v' \rangle_k \rangle_h = -\nu_{x,y} \left(\frac{\partial u_h}{\partial y} + \frac{\partial v_h}{\partial x} \right)$$

and

$$\langle v_h'^2 + \langle v'^2 \rangle_k \rangle_h = -2\nu_{y,y} \frac{\partial v_h}{\partial y}$$

However, these coefficients certainly are not the same as the coefficients of eddy viscosity which were employed in Section 1 of this chapter in the terms replacing the Reynolds stresses in the three-dimensional equations.

For the present we have no basis for relating these terms to known or computable parameters. Our best hope for the present is that, as they appear in the dynamic equations, the terms containing the vertical mean cross-products of the velocity deviations can be neglected. If this is so, then (2.62) and (2.63) become

$$\frac{\partial u_h}{\partial t} + u_h \frac{\partial u_h}{\partial x} + v_h \frac{\partial u_h}{\partial y} = -g \left\{ \frac{\partial \eta}{\partial x} + \langle i_{x,p,\eta} \rangle_h \right\} - \frac{1}{\rho_h} \frac{\partial p_a}{\partial x} + f v_h + \frac{1}{h\rho_h} \tau_{w,x} - g \frac{u_h (u_h^2 + v_h^2)^{\frac{1}{2}}}{h\, C_h^2} \tag{2.66}$$

and

$$\frac{\partial v_h}{\partial t} + u_h \frac{\partial v_h}{\partial x} + v_h \frac{\partial v_h}{\partial y} = -g \left\{ \frac{\partial \eta}{\partial y} + \langle i_{y,p,\eta} \rangle_h \right\} - \frac{1}{\rho_h} \frac{\partial p_a}{\partial y} - f u_h + \frac{1}{h\rho_h} \tau_{w,y} - g \frac{v_h (u_h^2 + v_h^2)^{\frac{1}{2}}}{h\, C_h^2} \tag{2.67}$$

Equations (2.21) and (2.22) from Section 1 of this chapter must be used as auxiliary equations to the above forms of the equation of motion in order that the relative isobaric slopes, $i_{x,p,\eta}$ and $i_{y,p,\eta}$, be computed from the distribution of density (salinity). Since the temporal changes in the distribution of salinity will alter the values of the relative isobaric slope, the equation expressing conservation of salt in two-dimensions, to be developed in the next sub-section, must be solved simultaneously with the equations of motion and the two-dimensional form of the equation of continuity of mass.

2.2.3 The Vertically Averaged Two-Dimensional Salt Balance Equation

Equation (2.30) given in Section 1 of this chapter, expressing the conservation of salt in three dimensions, serves as a starting point for this development of the vertically averaged salt balance equation. Omitting molecular diffusion, that equation is written in the notation used in this section as

$$\frac{\partial s}{\partial t} = -\frac{\partial}{\partial x}(us) - \frac{\partial}{\partial y}(vs) - \frac{\partial}{\partial z}(ws) - \frac{\partial}{\partial x}\langle u's'\rangle_k - \frac{\partial}{\partial y}\langle v's'\rangle_k - \frac{\partial}{\partial z}\langle w's'\rangle_k \qquad (2.68)$$

As was done in the treatment of continuity of mass and salt, we express the dependent variables as the sum of a vertical average plus a difference term. For example

$$s = s_h + s_h'$$

where

$$s_h = \frac{1}{h}\int_{-\xi}^{\eta} s \, dx_3 = \langle s\rangle_h$$

Integrating Equation (2.68) then gives

$$\begin{aligned}\frac{\partial (hs_h)}{\partial t} = &-\frac{\partial}{\partial x}(hu_h s_h) - \frac{\partial}{\partial y}(hv_h s_h) - \frac{\partial}{\partial x}\{h\langle u_h's_h' + \langle u's'\rangle_k\rangle_h\} \\ &- \frac{\partial}{\partial y}\{h\langle v_h's_h' + \langle v's'\rangle_k\rangle_h\} + s_h\,(E\text{-}P)\end{aligned} \qquad (2.69)$$

Again, this equation contains terms of the type $\langle u_h's_j'\rangle_h$, which have not normally been discussed in connection with existing two-dimensional models. These terms arise from the vertical shear in the horizontal velocity and the vertical gradient in salinity. We might argue that these terms can be replaced by a Fickian-type diffusion term as was done for terms of the type $\langle u's'\rangle_k$ in the three-dimensional case. That is, we might make the substitution

$$\begin{aligned}\langle u_h's_h' + \langle u's'\rangle_k\rangle_h &= -K_x^* \frac{\partial s_h}{\partial x} \\ \langle v_h's_h' + \langle v's'\rangle_k\rangle_h &= -K_y^* \frac{\partial s_h}{\partial y}\end{aligned} \qquad (2.70)$$

Then Equation (2.69) becomes

$$\begin{aligned}\frac{\partial (hs_h)}{\partial t} = &-\frac{\partial}{\partial x}(hu_h s_h) - \frac{\partial}{\partial y}(hv_h s_h) + \frac{\partial}{\partial x}\left\{hK_x^* \frac{\partial s_h}{\partial x}\right\} \\ &+ \frac{\partial}{\partial y}\left\{hK_y^* \frac{\partial s_h}{\partial y}\right\} + s_h\,(E\text{-}P)\end{aligned} \qquad (2.71)$$

coefficients such as K_x* and K_y* , which arise from terms involving shear in the velocity field and spatial gradients in the concentration distribution, are sometimes called "effective" diffusion coefficients. It is to be expected, however, that these coefficients will differ considerably from the eddy coefficients of diffusion which were introduced in the three-dimensional salt balance equations. There is also less justification for neglecting the diffusion terms in Equation (2.71) than for neglecting the horizontal viscous terms in the two-dimensional momentum equations. It is reasonable to assume, however, that $K_x* = K_y* = K_H*$, the "effective" horizontal diffusivity, and Equation (2.71) would then be written

$$\frac{\partial(hs_h)}{\partial t} = -\frac{\partial}{\partial x}[hu_h s_h] - \frac{\partial}{\partial y}[hv_h s_h] + \frac{\partial}{\partial x}\left\{hK_H*\frac{\partial s_h}{\partial x}\right\} + \frac{\partial}{\partial y}\left\{hK_H*\frac{\partial s_h}{\partial y}\right\} + s_h\,(E-P) \qquad (2.72)$$

The vertically averaged equation expressing the conservation of a dissolved or finely divided constituent, having sources and sinks in addition to those for salt, would then be written

$$\begin{aligned}\frac{\partial(h\zeta_H)}{\partial t} = &-\frac{\partial}{\partial x}[hu_h\zeta_h] - \frac{\partial}{\partial y}[hv_h\zeta_h] + \frac{\partial}{\partial x}\left\{hK_H*\frac{\partial\zeta_h}{\partial x}\right\}\\ &+\frac{\partial}{\partial y}\left\{hK_H*\frac{\partial\zeta_h}{\partial y}\right\} + \zeta_h\,(E-P) + hr_{g,h} - hr_{d,h}\end{aligned} \qquad (2.73)$$

where $r_{g,h}$ is the vertically averaged mass rate of generation of the constituent per unit volume (such as the discharge of a waste material) and $r_{d,h}$ is the vertically averaged mass rate of decay of the constituent per unit volume (such as oxidation of an organic waste).

2.2.4 Summary of the Set of Vertically Averaged Dynamic and Kinematic Equations Suitable to Serve as the Basis of a Two-Dimensional Numerical Model of an Estuary

The vertically averaged equation of mass continuity,

$$\frac{\partial(hu_h)}{\partial x} + \frac{\partial(hv_h)}{\partial y} = -\frac{\partial\eta}{\partial t} \qquad (2.59)$$

together with the somewhat simplified vertically averaged equations of motion, given by

$$\begin{aligned}\frac{\partial u_h}{\partial t} + u_h\frac{\partial u_h}{\partial x} + v_h\frac{\partial u_h}{\partial y} = &-g\left\{\frac{\partial\eta}{\partial x} + \langle i_{x,p,\eta}\rangle_h\right\} - \frac{1}{\rho_h}\frac{\partial p_a}{\partial x} + fv_h\\ &+\frac{1}{h\rho_h}\tau_{w,x} - g\,\frac{u_h(u_h^2 + v_h^2)^{\frac{1}{2}}}{h\,C_h^2}\end{aligned} \qquad (2.66)$$

and

$$\frac{\partial v_h}{\partial t} + u_h \frac{\partial v_h}{\partial x} + v_h \frac{\partial v_h}{\partial y} = -g \left\{\frac{\partial \eta}{\partial y} + \langle i_{y,p,\eta} \rangle_h\right\} - \frac{1}{\rho_h} \frac{\partial p_a}{\partial y} - f u_h$$

$$+ \frac{1}{h\rho_h} \tau_{w,y} - g \frac{v_h (v_h^2 + u_h^2)^{\frac{1}{2}}}{h\, C_h^2} \tag{2.67}$$

represent a set of three equations which could be solved simultaneously for the three dependent variables u_h, v_h and η, provided the necessary numerical values of the initial and boundary conditions are available. However, we note that the vertical averages of the relative isobaric slopes, $\langle i_{x,p,\eta} \rangle_h$ and $\langle i_{y,p,\eta} \rangle_h$, depend on the distribution of density and hence of salinity. Thus the vertically averaged salt balance equation,

$$\frac{\partial (h s_h)}{\partial t} = - \frac{\partial}{\partial x} (h u_h s_h) - \frac{\partial}{\partial y} (h v_h s_h) + \frac{\partial}{\partial x} \left\{h K_H^* \frac{\partial s_h}{\partial x}\right\} + \frac{\partial}{\partial y} \left\{h K_H^* \frac{\partial s_h}{\partial y}\right\} + s_h (E-P) \tag{2.72}$$

must be solved simultaneously with Equations (2.59), (2.66) and (2.67) to provide the horizontal distribution of salinity. As discussed in Section 1 of this chapter, the horizontal distribution of salinity thus determined can be combined with an assumed distribution of temperature to compute the horizontal distribution of density. The vertical mean values of the relative isobaric slope terms $\langle i_{x,p,\eta} \rangle_h$ and $\langle i_{y,p,\eta} \rangle_h$ can then be determined from the relationships (obtained by taking the vertical average of Equation 2.20 from Section 1 of this chapter)

$$\langle i_{x,p,\eta} \rangle_h = \tfrac{1}{2} (\eta+\xi) \cdot \frac{1}{\rho_h} \frac{\partial \rho_h}{\partial x} = \tfrac{1}{2} (\eta+\xi) \frac{10^{-3}}{1+10^{-3}\sigma_t} \frac{\partial \sigma_t}{\partial x} \tag{2.74}$$

and

$$\langle i_{y,p,\eta} \rangle_h = \tfrac{1}{2} (\eta+\xi) \cdot \frac{1}{\rho_h} \frac{\partial \rho_h}{\partial y} = \tfrac{1}{2} (\eta+\xi) \frac{10^{-3}}{1+10^{-3}\sigma_t} \frac{\partial \sigma_t}{\partial y} \tag{2.75}$$

The required inputs for numerical solution of Equations (2.59), (2.66), (2.67) and (2.72) are: (a) the physical dimensions of the estuary; (b) the temporal and spatial distribution of atmospheric pressure and of surface wind stress over the period covered by the computations; (c) the fresh water inflow to the estuary as a function of time during the period covered by the computations; (d) values of the difference, evaporation minus precipitation, at the water surface of the estuary as a function of horizontal position and time during the period covered by the computations; (e) an assumed horizontal distribution of vertical-averaged water temperature in the estuary; (f) values of the Chezy resistance coefficient as a function of position in the estuary; (g) values of the effective horizontal diffusivity as a function of position in the estuary and of time over the period covered by the computations; (h) values of the surface elevation η and of the vertically averaged salinity s_h along a line marking the seaward boundary of the estuary, as a function of time during the period covered by the computations; (i) an initial set of values of the dependent variables at all positions in the estuary.

The dependent variables to be computed from the numerical solution of these equations are: (a) the surface elevation, η ; (b) the vertically averaged horizontal components of the velocity, u_h and v_h ; and (c) the vertically averaged salinity s_h ; all as functions of horizontal position (x, y) and of time over the period of the computations. Equations (2.74) and (2.75) must be used as auxiliary equations of the computations to obtain values of the vertically averaged relative isobaric slopes $\langle i_{x,p,\eta}\rangle_h$ and $\langle i_{y,p,\eta}\rangle_h$ from the computed distribution of salinity and the assumed distribution of temperature. The additional integral condition, obtained from the integration of the vertically averaged equation of continuity across the estuary and then along the estuary from the landward boundary of the estuary $(x = x_o)$, where the time variation in water surface elevation is zero, must also be satisfied. That is,

$$\int_b hu_h dy = Q_R - \frac{\partial}{\partial t}\left\{\int_{x_o}^{x} \sigma \, dx'\right\} \qquad (2.76)$$

where $\int_b dy$ indicates an integral across the width of the estuary $b(x,t)$; and $\sigma(x,t)$ is the cross-sectional area of the estuary perpendicular to the x-axis, which is considered here to be oriented along the estuary.

2.2.5 An Alternate Development of a Set of Vertically Averaged Dynamic and Kinematic Equations in an Estuary

Jan J. Leendertse (personal communication) has suggested an alternate approach to the development of the vertically averaged equations which offers some computational advantages over the development given above. Briefly, this approach is based on the assumption that the ensemble mean velocity components, $u(x,y,z,t)$ and $v(x,y,z,t)$, and salinity $s(x,y,z,t)$ are related to their respective vertical-averaged values $u_h(x,y,t)$, $v_h(x,y,t)$, and $s_h(x,y,t)$ by the relationships

$$u = u_h\,\{1 + f_u(z)\}$$

$$v = v_h\,\{1 + f_v(z)\} \qquad (2.77)$$

and

$$s = s_h\,\{1 + f_s(z)\}$$

where $f_u(z)$, $f_v(z)$ and $f_s(z)$ are functions of the vertical coordinate z , and also perhaps of the time t , and describe all the vertical variations in u , v , and x , respectively. Note that this manner of relating the ensemble mean values of the variables to their respective vertical-averaged values is more restrictive than the division given in Equation (2.53), since Equation (2.77) requires that u, v and s are zero everywhere in the vertical when their respective vertical mean values u_h, v_h and s_h are zero, a condition not generally true.

The vertical integrals of the functions $f_u(z)$, $f_v(z)$ and $f_s(z)$ must all be zero. However, cross-products involving these functions do not necessarily have vertical averages equal to zero. The integral cross-products which appear in the vertically averaged equations are

$$\int_{-\xi}^{\eta} u^2\, dz = u_h^2 \int_{-\xi}^{\eta} \{1 + f_u(z)\}^2\, dz$$

$$= u_h^2 \int_{-\xi}^{\eta} \{1 + f_u^2(z)\}\, dz \qquad (2.78)$$

$$\int_{-\xi}^{\eta} uv\,dz = u_h v_h \int_{-\xi}^{\eta} \{1 + f_u(z)\}\{1 + f_v(z)\}\,dz$$

$$= u_h v_h \int_{-\xi}^{\eta} \{1 + f_u(z)\cdot f_v(z)\}\,dz \tag{2.79}$$

$$\int_{-\xi}^{\eta} us\,dz = u_h s_h \int_{-\xi}^{\eta} \{1 + f_u(z)\}\{1 + f_s(z)\}\,dz$$

$$= u_h s_h \int_{-\xi}^{\eta} \{1 + f_u(z)\ f_s(z)\}\,dz \tag{2.80}$$

and

$$\int_{-\xi}^{\eta} vs\,dz = v_h s_h \int_{-\xi}^{\eta} \{1 + f_v(z)\}\{1+f_s(z)\}\,dz$$

$$= v_h s_h \int_{-\xi}^{\eta} \{1 + f_v(z)\cdot f_s(z)\}dz \tag{2.81}$$

Now designate

$$\alpha_{uu} = \frac{1}{h}\int_{-\xi}^{\eta} \{1 + f_u^{2}(z)\}dz \tag{2.82}$$

$$\alpha_{uv} = \frac{1}{h}\int_{-\xi}^{\eta} \{1 + f_u(z)\cdot f_v(z)\}\,dz \tag{2.83}$$

$$\alpha_{us} = \frac{1}{h}\int_{-\xi}^{\eta} \{1 + f_u(z)\cdot f_s(z)\}\,dz \tag{2.84}$$

and

$$\alpha_{vs} = \frac{1}{h}\int_{-\xi}^{\eta} \{1 + f_v(z)\cdot f_s(z)\}\,dz \tag{2.85}$$

where α_{uu}, α_{uv}, α_{us}, and α_{vs} are called the distribution functions for the respective cross-products which define them. Hopefully, the spatial, and perhaps temporal variations in these parameters are sufficiently regular to be revealed from observations of the vertical variation in the velocity and salinity in the estuary. The uncertainties in these parameters substitute for the uncertainties in the effective horizontal coefficients of viscosity and diffusivity. Hopefully, however, the variations in these in space and time would be more readily related to known parameters than in the case of the effective coefficients.

In any case, the vertically averaged equation of continuity has the same form in this development as that given earlier. That is, Equation (2.59) remains applicable. The vertically averaged equations of motion become, however,

$$\frac{\partial(hu_h)}{\partial t} + \frac{\partial(h\alpha_{uu}u_h^{2})}{\partial x} + \frac{\partial(h\alpha_{uv}u_h v_h)}{\partial y} = -gh\,\frac{\partial\eta}{\partial x} - gh\,\langle i_{x,p,\eta}\rangle_h - \frac{h}{\rho_h}\frac{\partial p_a}{\partial x}$$

$$+fhv_h + \frac{1}{\rho_h}\,\tau_{w,x} - g\,\frac{u_h(u_h^{2}+v_h^{2})^{\frac{1}{2}}}{C_h^{2}} \tag{2.86}$$

and

$$\frac{\partial(hv_h)}{\partial t} + \frac{\partial(h\alpha_{uv}u_h v_h)}{\partial x} + \frac{\partial(h\alpha_{vv}{v_h}^2)}{\partial y} = -gh\,\frac{\partial\eta}{\partial y} - gh\,\langle i_{y,p,\eta}\rangle_h - \frac{h}{\rho_h}\frac{\partial p_a}{\partial y}$$

$$- fhu_h + \frac{1}{\rho_h}\,\tau_{w,y} - g\,\frac{v_h({u_h}^2+{v_h}^2)^{\frac{1}{2}}}{{C_h}^2} \qquad (2.87)$$

where the vertical average of the ensemble mean cross-product terms involving the turbulent velocity deviations, such as $\langle u'v'\rangle_k$, have been neglected. There is considerably greater justification for neglecting these terms in the development of Equations (2.86) and (2.87) than for neglecting terms such as $\langle u_h'v_h' + \langle u'v'\rangle_k\rangle_h$ as was done in arriving at Equations (2.66) and (2.67). Essentially, the distribution functions α_{uu}, α_{vv} and α_{uv} take the place of cross-products of the type $\langle u_h'v_h'\rangle_h$. Thus Equations (2.86) and (2.87) are at least conceptually more complete than Equations (2.66) and (2.67). The somewhat restrictive relationship between u and u_h, etc., as given in Equation (2.77) must, however, be kept in mind in making this comparison.

The vertically averaged salt balance equation, using the relationships given in Equation (2.77), then becomes

$$\frac{\partial(hs_h)}{\partial t} = -\frac{\partial}{\partial x}(h\alpha_{us}u_h s_h) - \frac{\partial}{\partial y}(h\alpha_{vs}v_h s_h) + \frac{\partial}{\partial x}\left\{h\,\bar{K}_H\,\frac{\partial s_h}{\partial x}\right\}$$

$$+ \frac{\partial}{\partial y}\left\{h\,\bar{K}_H\,\frac{\partial s_h}{\partial y}\right\} + s_h\,(E-P) \qquad (2.88)$$

where the diffusion terms arise from the substitution

$$\langle\langle u's'\rangle_k\rangle_h = -\bar{K}_H\,\frac{\partial s_h}{\partial x}$$

and

$$\langle\langle u's'\rangle_k\rangle_h = -\bar{K}_H\,\frac{\partial s_h}{\partial y}$$

The vertically averaged horizontal diffusivity $\bar{K}_H$ is thus probably much smaller than the effective horizontal diffusivity $K_H{}^*$ which appears in Equation (2.72), since the latter coefficient arose from a substitution of the form given in Equation (2.70).

This alternate approach provides a model less dependent on our lack of knowledge of the effective horizontal coefficients of viscosity and diffusivity. However, in place of the need for finding relationships between these coefficients and known parameters, it is necessary to define the spatial and temporal variations in the distribution functions α_{uu}, α_{vv}, α_{uv}, α_{us}, and α_{vs}. Certainly the observational requirements for establishing empirical relationships for the distribution functions are less severe than in the case of the effective horizontal coefficients of viscosity and diffusivity. On the basis of available evidence, the distribution functions will, for most estuaries, and for most times during the tidal cycle, range between 0.5 and 1.5. The more nearly the estuary is vertically homogeneous in velocity and salinity, the closer the distribution functions will be to unity.

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3. ONE-DIMENSIONAL MODELS

Donald R. F. Harleman

3.1 INTRODUCTION

One-dimensional equations for the hydrodynamic and mass transfer processes in estuaries have an obvious advantage of mathematical tractability in comparison with their multi-dimensional counterparts. In addition, the one-dimensional equations utilize and predict information that is related to available or accessible observational data. This is especially true in dealing with the mass transfer equations for water quality parameters involving source and sink terms, such as biochemical oxygen demand and dissolved oxygen.

An important objective of this section is the presentation, comparison and discussion of the various one-dimensional hydrodynamic and mass transfer models which have been used in estuaries. Thus it is necessary to consider the most general form of these equations in which quantities such as concentration and velocity are functions of both longitudinal position and real time. The general equations are employed as the basis for evaluation of simpler mathematical models which use non-tidal advective velocities.

The one-dimensional mass transfer equation is derived by a spatial integration of the three-dimensional equation over the flow cross section. Thus any quantities such as velocity, concentration or dissolved oxygen are spatial averages over a cross section corresponding to a specified period of time averaging. The one-dimensional continuity and momentum equations are derived by considering a material element occupying a cross section of the estuary. The one-dimensional equations are well suited for estuaries displaying vertical and lateral homogeneity; however, they have been successfully applied to estuaries with varying degrees of sectional non-homogeneity. Applications to a fully stratified or saline-wedge estuary should be excluded. The latter problems can be treated by the theory of two-layer stratified flows (Harleman 1960, Keulegan 1966).

The various quantities, such as velocity, concentration, cross-sectional area, in the one-dimensional mathematical models are assumed to be functions of a single spatial variable x and time t. The longitudinal distance x is measured along the axis of the estuary and cross-sectional areas are normal to the local direction of the axis as shown in Figure 2.1.

One-dimensional mathematical models encompass a wide range of time-averaging concepts. This has been the subject of confusion in the literature due to the use of ambiguous terms for time averaging. Adjectives such as "unsteady", "quasi-steady state" or "steady" are meaningless unless precisely defined with respect to (i) the duration of the time period to be used in averaging, and (ii) the quantity to which the adjective applies. Careful definition is particularly important in estuarine problems because of the multitude of time-averaging concepts which have been employed. As shown in Figure 2.2, the term "unsteady" when applied to the section-mean velocity may imply as many as four possible periods of time averaging. These are defined as follows:

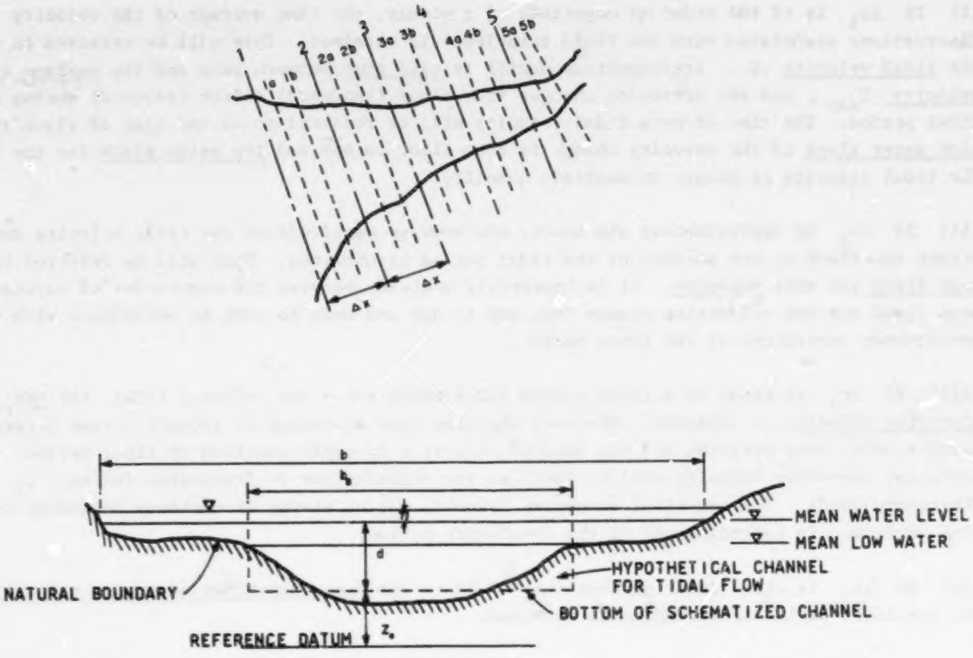

1
1a
1b
2
2a
2b
3
3a
3b
4
4a
4b
5
5a
5b
Δx
Δx
b
b_s
h
d
MEAN WATER LEVEL
MEAN LOW WATER
HYPOTHETICAL CHANNEL
FOR TIDAL FLOW
NATURAL BOUNDARY
BOTTOM OF SCHEMATIZED CHANNEL
REFERENCE DATUM
z_o

Fig. 2.1 Longitudinal and transverse schematization of an estuary.

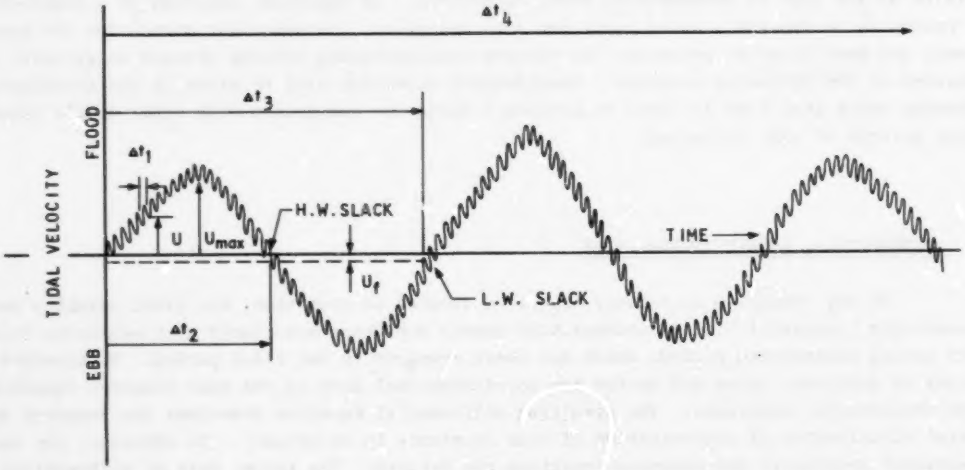


Fig. 2.2 Various periods of time-averaging the tidal velocity.

(i) If Δt_1 is of the order of magnitude of a minute, the time average of the velocity fluctuations associated with the fluid turbulence is obtained. This will be referred to as the tidal velocity U. Its magnitude varies in real time between zero and the maximum tidal velocity U_{max}, and the direction changes from flood (landward) to ebb (seaward) during each tidal period. The time of zero tidal velocity will be referred to as the time of slack tide; high water slack if the velocity change is from flood to ebb and low water slack for the reverse. The tidal velocity is always an unsteady quantity.

(ii) If Δt_2 is approximately six hours, the average magnitude of the tidal velocity during either the flood or ebb portion of the tidal period is obtained. This will be referred to as mean flood (or ebb) velocity. It is inherently unsteady because the magnitudes of successive mean flood and ebb velocities change from day to day and week to week in accordance with the spring-neap variations of the lunar month.

(iii) If Δt_3 is equal to a tidal period (12.4 hours for a semi-diurnal tide), the non-tidal advective velocity is obtained. Whenever the time rate of change of estuary volume between the section under consideration and the head of tide is a harmonic function of tidal period, the non-tidal advective velocity will be equal to the velocity due to freshwater inflow, U_f (Pritchard 1958). The non-tidal advective velocity may be steady or unsteady depending on the time variation in the magnitude of the freshwater inflow.

(iv) If Δt_4 is equal to or greater than 25 hours the mean, non-tidal advective velocity for the specified period of averaging is obtained.

Time-averaging terms may be applied to quantities other than velocity and care should be taken to specify the intention. For example, consider the instantaneous or pulse injection of a tracer into a steady, uniform flow. In this case the velocity is steady, however the concentration at a fixed point is a function of time and is therefore unsteady.

The various one-dimensional mathematical models employed in analysis of pollution problems in estuaries can be classified according to the length of the time averaging associated with the advective velocity. It is essential that good judgement be used in arriving at the decision of the type of mathematical model to be used. An important function of a state-of-the-art review is to provide a sound basis for such decisions. Mathematical models for the hydrodynamic and mass transfer processes for various time-averaging periods related to velocity are presented in the following sections. Considerable attention will be given to the development of models using real time in order to provide a basis for comparison with other models using longer periods of time averaging.

3.2 MATHEMATICAL MODELS IN REAL TIME

If the events in an estuary are to be treated in real time, the tidal velocity and concentration quantities in the mathematical models are those associated with measuring instruments having integrating periods which are short compared to the tidal period. We consider an estuary of arbitrary shape and derive the one-dimensional form of the mass transfer equation for a non-conservative substance. The resulting differential equation describes the temporal and spatial distribution of concentration of that substance in an estuary. In addition, the one-dimensional continuity and momentum equations are derived. The latter pair of differential equations may be used to determine the tidal velocity which appears in the advective term of the mass transfer equation.

3.2.1 Mass Transfer Equation for a Non-Conservative Substance

The one-dimensional mass transfer equation can be obtained by direct integration of the three-dimensional equation over a cross section normal to the axis of the estuary. The three-dimensional equation for turbulent flow, neglecting molecular diffusion is

$$\frac{\partial c}{\partial t} + u\frac{\partial c}{\partial x} + v\frac{\partial c}{\partial y} + w\frac{\partial c}{\partial z} = \frac{\partial}{\partial x}\left(e_x\frac{\partial c}{\partial x}\right) + \frac{\partial}{\partial y}\left(e_y\frac{\partial c}{\partial y}\right) + \frac{\partial}{\partial z}\left(e_z\frac{\partial c}{\partial z}\right) + r_i/\rho \qquad (2.89)$$

where u, v, w are the time-averaged velocity components associated with turbulent flow, c is the local concentration, e_x, e_y and e_z are turbulent diffusivities, and r_i is the time rate of generation (or decay) of substance per unit volume of fluid. We define

$$\begin{aligned} u &= U + u'' \\ v &= v'' \\ w &= w'' \end{aligned} \qquad (2.90)$$

where $U = \frac{1}{A}\int_A u\,dA$ is the real time longitudinal tidal velocity averaged over the cross section. The double-primed quantities u'', v'' and w'' are spatial deviations of velocity from the section-mean value due to the vertical and lateral velocity distribution. Note that

$$\int_A u''\,dA = 0$$

and that v'' and w'' are not zero even though the section-mean velocities V and W are zero in a one-dimensional flow. In a similar manner, we define

$$c = C + c'' \qquad (2.91)$$

where $C = \frac{1}{A}\int_A c\,dA$ is the concentration averaged over the cross section and c'' is the spatial deviation of the concentration due to the variation of concentration over the cross section. Concentration is defined as the mass of substance per unit mass of solution (or weight of substance per unit weight of solution).

Equations (2.90) and (2.91) are introduced into the three-dimensional mass transfer Equation (2.89), the products of sums are expanded and each term is integrated over the cross-sectional area A. Inasmuch as the expanded equation contains at least thirteen terms a complete development will not be presented. Rigorous derivations of this type have been given by Okubo (1964) and Holley and Harleman (1965). After simplification, the one-dimensional equation may be written as

$$\frac{1}{A}\frac{\partial(AC)}{\partial t} + \frac{1}{A}\frac{\partial}{\partial x}(AUC) + \frac{1}{A}\frac{\partial}{\partial x}\int_A u''c''\,dA = \frac{1}{A}\frac{\partial}{\partial x}\left(A\bar{e}_x\frac{\partial C}{\partial x}\right) + \frac{r_i}{\rho} + \frac{r_e}{\rho} \qquad (2.92)$$

The integral term on the left side involving the cross product of the longitudinal velocity and concentration deviations represents the mass transport associated with the non-uniform velocity distribution. This is usually designated as the longitudinal dispersion term. The quantity $\bar{e}_x$

is the spatial-mean value of the turbulent diffusivity. The term r_i represents the time rate of internal addition of mass per unit volume by generation of the substance within the fluid. The term r_e is the time rate of addition of mass per unit volume externally across the lateral boundaries (sides, bottom and water surface). The two latter quantities are usually known as source and sink terms. As examples of internal terms, a positive r_i would result from oxygen produced by suspended algae; and r_i would be negative for a substance undergoing radioactive decay or for the consumption of oxygen by suspended matter possessing BOD. In the case of mass transfer across external boundaries, a positive value of r_e could be due to the absorption of atmospheric oxygen across the free surface of an oxygen deficient stream. A negative r_e would result from the adsorption of a tracer dye on the solid boundaries.

For steady, uniform flow, Taylor (1954) and Aris (1956) have shown that the advective mass transport associated with the cross product of the spatial deviations u'' and c'' can be represented as an analogous one-dimensional diffusive transport. To distinguish this process from turbulent diffusion, which is associated with the temporal deviations u' and c', the transport due to spatial deviations is called longitudinal dispersion. On this basis a coefficient of dispersion E is defined in terms of the concentration gradient as

$$\int_A u''c'' \, dA = - AE \frac{\partial C}{\partial x} \tag{2.93}$$

The negative sign indicates mass transport in the direction of decreasing concentration. Taylor (1954) has shown that E is more than two orders of magnitude larger than $\bar{e}_x$; therefore it is convenient to add the two coefficients and refer to the sum as the longitudinal dispersion coefficient E_L , where

$$E_L = E + \bar{e}_x \tag{2.94}$$

Using Equations (2.93) and (2.94), Equation (2.92) becomes

$$\frac{1}{A} \frac{\partial}{\partial t} (AC) + \frac{1}{A} \frac{\partial}{\partial x} (AUC) = \frac{1}{A} \frac{\partial}{\partial x} \left(AE_L \frac{\partial c}{\partial x}\right) + \frac{r_i}{\rho} + \frac{r_e}{\rho} \tag{2.95}$$

Equation (2.95) is the most general form of the one-dimensional mass transfer for a non-conservative substance. It is assumed to be valid for unsteady, non-uniform flows within the restrictions of the one-dimensional approximation. The independent variables, tidal velocity U , cross-sectional area A , and longitudinal dispersion coefficient E_L can be functions of both x and t . In addition, the source and sink terms can be functions of x and t . The dependent variable, concentration, refers to any substance of interest. In general, one mass transfer equation of the form of Equation (2.95) must be written for each substance under consideration. Typically, mass transfer equations are written for salinity, dye or radioactive tracers, BOD and dissolved oxygen.

The following discussions refer specifically to the various terms in the mass transfer equation.

3.2.2 Source and Sink Terms

The nature of the internal and external source and sink terms in the mass transfer Equation (2.95) depends on the substance under consideration. Their specification in quantitative terms is probably one of the most difficult problems in water quality modeling; this is treated in detail in Chapter III.

A substance is called conservative if the source and sink terms r_i and r_e are both zero. For example, salinity is usually considered to be a conservative substance in an estuary, in that the source of salinity is specified as a maximum concentration at the ocean end. The term $r_i = 0$ since no salinity is generated internally within an estuary and $r_e = 0$ if there is no influx of salinity along the external lateral boundaries.

The following discussion will serve to illustrate the proper dimensional form for two typical source and sink terms. A common sink term of the internal type is a decay which follows a so-called first-order reaction. This would be appropriate if the substance under consideration were a radioactive tracer. The first-order reaction is stated as follows: the time rate of decay (or generation) of a substance per unit volume (r_i) is directly proportional to the mass of the substance per unit volume present at any instant of time (ρC). Thus, for decay,

$$r_i = - K_d(\rho C) \tag{2.96}$$

and the sink term in Equation (2.95) is

$$\frac{r_i}{\rho} = - K_d C \tag{2.97}$$

where K_d is the reaction coefficient in units of t^{-1}.

A common source term of the external type arises from the transfer of oxygen from the atmosphere across the free surface of a fluid having the capacity to increase its dissolved oxygen content. The following statement expresses the film theory concept (Dobbins 1964) of oxygen transfer: the time rate of increase in the mass of dissolved oxygen per unit volume (r_e) is directly proportional to the product of the free surface area per unit volume and the deficit in the mass of dissolved oxygen per unit volume in the liquid phase. This assumes no vertical gradient in the concentration of dissolved oxygen within the fluid except for a film of molecular thickness at the free surface. Thus

$$\frac{\text{increase in mass of DO}}{(\text{volume})\ \ (\text{time})} = K_L \left[\frac{A_s}{(\text{volume})}\right] \left[\frac{\text{mass of DO at saturation}}{(\text{volume})} - \frac{\text{mass of DO}}{(\text{volume})}\right] \tag{2.98}$$

where K_L is the film coefficient (L/t) of oxygen transfer and A_s is the free surface area. Multiplying and dividing the right-hand side by the fluid density results in

$$r_e = \rho K_L \frac{A_s}{(\text{volume})} [C_s - C] \tag{2.99}$$

where C_s is the saturation concentration of dissolved oxygen. The ratio of surface area to volume can be interpreted as the reciprocal of the mean depth d and the combination K_L/d is usually known as the reaeration coefficient K_a. Therefore the source term in Equation (2.95) is

$$\frac{r_e}{\rho} = K_a\ (C_s - C) \tag{2.100}$$

Both K_a and K_d may be functions of x and t .

3.2.3 Tidal Velocity

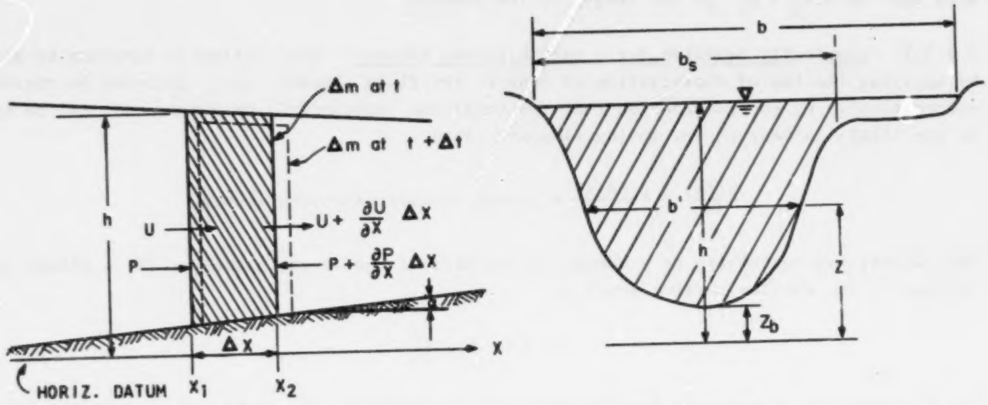
The tidal velocity term (U) in the mass transfer equation can be obtained in a number of ways. The choice depends on available data and the accuracy desired in describing the advective motion in the estuary. It should be emphasized that the advective motion and the source and sink terms are usually the dominant quantities in the mass transfer equation. The dispersion term is related to the spatial variations of the actual advective velocities from the sectional-mean value U in the one-dimensional equation. Thus the importance of the dispersion term decreases as the accuracy of the description of the advective process increases. This is important because the dispersion coefficient has been one of the most elusive quantities in water quality mathematical models.

Significant advances in the analysis and calculation of tidal motion in estuaries have been made in recent years. Therefore it is technically feasible to incorporate the knowledge of tidal motion into the analysis of estuarine water quality. Improvements in the hydrodynamic aspects of water quality models are a prerequisite to a systematic investigation of the magnitude of the various source and sink terms for estuaries.

The tidal velocity can be obtained (i) by direct measurement of tidal velocities in an estuary, (ii) by measurement of tidal elevations and calculation of tidal velocity through the continuity equation, or (iii) by a combined solution of the continuity and momentum equations. The latter requires only the specification of estuary geometry and certain boundary conditions, and it is therefore the only method which can be used for predictive purposes. The appropriate one-dimensional continuity and momentum equations are derived in the following sections.

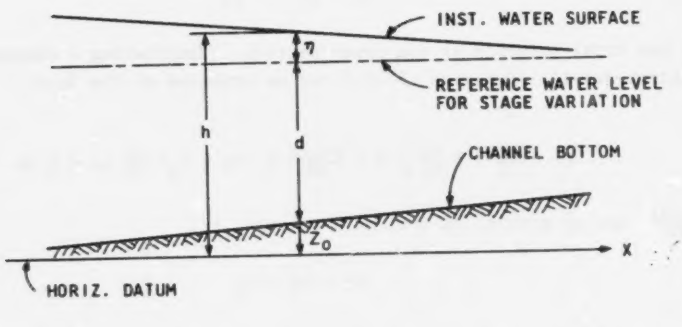
A cross section of an irregular estuary is shown in Figure 2.3. The x-coordinate is measured horizontally along the longitudinal axis from the ocean end of the estuary, and h is the distance to the instantaneous position of the water surface from a horizontal reference datum. The flow is assumed to be one-dimensional, hence channel curvature and Coriolis effects are neglected and the transverse water surface is horizontal. The density is assumed to be constant, and hydrostatic pressure is assumed to prevail at all points in the flow.

Within the Eulerian viewpoint, the one-dimensional conservation of volume (continuity) and momentum equations may be formulated in either of two ways: the *material* method or the *control volume* method. In the *material* method the flow characteristics at a section are obtained by following the motion of a *given mass of fluid* Δm through a small increment of time Δt in the vicinity of a fixed section. In the *control volume* method, the equations are derived by considering the *flux of mass and momentum* through a fixed control volume. The one-dimensional momentum equation is most readily derived by means of the material method, whereas the continuity equation is usually derived by the control volume method. In order to be consistent, the material method will be used for both developments. Derivations of the continuity and momentum equations for variable area tidal channels have also been given by Stoker (1957), Dronkers (1964), Lai (1965), and Harleman and Lee (1969).



Δm at t
Δm at $t + \Delta t$
h
U
$U + \frac{\partial U}{\partial X} \Delta X$
P
$P + \frac{\partial P}{\partial X} \Delta X$
Z
ΔX
X
HORIZ. DATUM
X_1
X_2
b
b_s
b'
h
Z
Z_b

Fig. 2.3 Definition sketch - Irregular channel.



INST. WATER SURFACE
η
REFERENCE WATER LEVEL FOR STAGE VARIATION
h
d
CHANNEL BOTTOM
Z_o
X
HORIZ. DATUM

Fig. 2.4 Definition sketch - Rectangular channel.

If, as shown in Figure 2.3, the section has both deep and very shallow portions, the cross section may be divided into conveyance and storage regions. In this case the tidal flow is assumed to be confined to the conveyance area defined by the width b_s , and the shallow portion defined by the width $b - b_s$ contributes to storage only. The cross-sectional area A is defined as the area of the conveyance section. Hence, the section-average tidal velocity $U = Q/A$, where Q is the instantaneous discharge through the section. The fluid mass Δm at time t is shown in Figure 2.3 by the planes at x_1 and x_2 . The mass of water in motion at time t is given by $\rho A \Delta x$, in which ρ is the density of water, A is the cross-sectional area and $\Delta x = x_2 - x_1$ is the length of the element.

3.2.3.1 Continuity Equation for a Variable Area Estuary The continuity equation is derived by applying the law of conservation of mass to the fluid element Δm . This may be expressed mathematically by the requirement that the total (or substantial) derivative of Δm be equal to the change in mass of the moving element. Thus

$$\frac{D(\Delta m)}{Dt} = \frac{D(\rho A \Delta x)}{Dt} = \text{change in mass of moving element}$$

Two factors may contribute to a change in the mass of the moving element: (1) a change due to storage in the shallow portion equal to

$$- \rho (b - b_s) \frac{\partial h}{\partial t} \Delta x$$

(2) a change due to external lateral flow into the element (caused by tributary inflow, spillage over a levee or seepage through the channel bank) equal to

$$\rho \; q \; \Delta x$$

where q is the lateral discharge per unit of longitudinal length (positive for inflow and negative for outflow). Thus the continuity equation can be written

$$\frac{D(\rho A \Delta x)}{Dt} = - \rho (b - b_s) \frac{\partial h}{\partial t} \Delta x + \rho \; q \; \Delta x \tag{2.101}$$

The total derivative can be expressed in terms of partial derivatives through the relation

$$\frac{D}{Dt} = \frac{\partial}{\partial t} + U \frac{\partial}{\partial x} \tag{2.102}$$

where U is the tidal velocity at the cross section. Considering a homogeneous, incompressible fluid of constant density, Equation (2.101) can be expanded to the form

$$\Delta x \left(\frac{\partial A}{\partial t} + U \frac{\partial A}{\partial x} \right) + A \frac{D(\Delta x)}{Dt} = -(b - b_s) \frac{\partial h}{\partial t} \Delta x + q \; \Delta x \tag{2.103}$$

The term $\frac{D(\Delta x)}{Dt}$ may be treated as follows: at time t ,

$$\Delta x = x_2 - x_1$$

at time $t + \Delta t$,

$$\Delta x' = x_2 + \left(U + \frac{\partial U}{\partial x}\Delta x\right)\Delta t - (x_1 + U\,\Delta t)$$

or

$$\Delta x' = x_2 - x_1 + \frac{\partial U}{\partial x}\Delta x\Delta t$$

Therefore,

$$\frac{D(\Delta x)}{Dt} = \frac{\Delta x' - \Delta x}{\Delta t} = \frac{\partial U}{\partial x}\Delta x \qquad (2.104)$$

and Equation (2.103) becomes, after dividing by Δx ,

$$\frac{\partial A}{\partial t} + U\frac{\partial A}{\partial x} + A\frac{\partial U}{\partial x} + (b - b_s)\frac{\partial h}{\partial t} - q = 0$$

or, since the discharge $Q = AU$,

$$\frac{\partial A}{\partial t} + \frac{\partial Q}{\partial x} + (b - b_s)\frac{\partial h}{\partial t} - q = 0 \qquad (2.105)$$

Referring to Figure 2.3, where the moving stream surface width $b_s = \partial A/\partial h$, it follows that

$$\frac{\partial A}{\partial t} = \frac{\partial A}{\partial h}\frac{\partial h}{\partial t} = b_s\frac{\partial h}{\partial t}$$

and Equation (2.105) becomes

$$b\frac{\partial h}{\partial t} + \frac{\partial Q}{\partial x} - q = 0 \qquad (2.106)$$

Equation (2.106) is known as the continuity equation.

3.2.3.2 Momentum Equation for a Variable Area Estuary The equation of motion is derived from Newton's Second Law, in the momentum equation form, which states that the time rate of change of longitudinal momentum is equal to the sum of external longitudinal forces acting on the moving fluid element. The longitudinal momentum is given by the product

$$(\Delta m)U = (\rho A\Delta x)\frac{Q}{A} = \rho Q\Delta x$$

The time rate of change of momentum is given by the total derivative which is equated to the summation of forces $\sum F_x$ to obtain the momentum equation

$$\frac{D(\rho Q\Delta x)}{Dt} = \rho\Delta x\frac{DQ}{Dt} + \rho Q\frac{D(\Delta x)}{Dt} = \sum F_x \qquad (2.107)$$

From Equations (2.102) and (2.104)

$$\frac{DQ}{Dt} = \frac{\partial Q}{\partial t} + U \frac{\partial Q}{\partial x} \quad \text{and} \quad \frac{D(\Delta x)}{Dt} = \frac{\partial U}{\partial x} \Delta x$$

and Equation (2.107) becomes

$$\rho \Delta x \left(\frac{\partial Q}{\partial t} + U \frac{\partial Q}{\partial x}\right) + \rho Q \frac{\partial U}{\partial x} \Delta x = \sum F_x \tag{2.108}$$

The possibility of a change in the longitudinal momentum flux due to flow entering or leaving the main channel from the storage area and due to the lateral inflow q has been discussed by various investigators. This involves an inherent assumption as to the direction in which the flow enters or leaves the conveyance section. As pointed out by Dronkers (1964, p. 194), the momentum effect also depends on whether the water level is rising or falling. It is generally agreed that the effect on the momentum equation is small, hence in this development it will be assumed that the lateral flows enter or leave the main channel at right angles to the longitudinal axis and that there is no contribution to the longitudinal momentum flux.

The correction to the longitudinal momentum flux due to the non-uniform velocity distribution at a cross section has also been neglected in this development. The momentum correction factor is usually of the order of three to five percent. The possibility of schematization of the cross section into conveyance and storage regions is an approximate method of accounting for highly non-uniform velocity distributions, and further refinements concerning the velocity distribution are not warranted.

The summation of external forces $\sum F_x$ consists of P, the resultant hydrostatic pressure force on the vertical cross section; $(P_w)_x$, the x-component of the horizontal pressure force exerted by the converging boundaries of the section; $(F_f)_x$, the frictional resistance force exerted by the boundaries. Hence, the three forces, using the notation shown in Figure 2.3, are

$$\sum F_x = \left[P - (P + \frac{\partial P}{\partial x} \Delta x) \right] + (P_w)_x - (F_f)_x$$

or

$$\sum F_x = - \frac{\partial P}{\partial x} \Delta x + (P_w)_x - (F_f)_x \tag{2.109}$$

The total pressure force on a vertical face is

$$P = \int_{z_b}^{h} \rho g(h - z)b'dz$$

where b' is the channel width at elevation z. Hence, by the use of Leibnitz' rule

$$\frac{\partial P}{\partial x} = \rho g \frac{\partial h}{\partial x} A + \rho g \int_{z_b}^{h} (h - z) \frac{\partial b'}{\partial x} dz \tag{2.110}$$

where the flow area $A = \int_{z_b}^{h} b'dz$. The boundary pressure force is

$$(P_w)_x = \rho g \int_{z_b}^{h} (h - z) \frac{\partial b'}{\partial x} \Delta x \, dz \tag{2.111}$$

The average frictional shear stress on the boundary of the element is

$$\tau_o = \rho g \, R S_E$$

where R is the hydraulic radius, $R = A/P_r$, P_r is the wetted perimeter and S_E is the slope of the energy gradient. The frictional force is therefore

$$F_f = \tau_o (P_r \Delta x) = \rho g \, A S_E \, \Delta x \tag{2.112}$$

The x-component may be taken equal to F_f since cos α ≈ 1. The slope of the energy gradient is evaluated from the Chezy equation in which

$$S_E = \frac{U|U|}{C_h^2 R} = \frac{Q|Q|}{A^2 C_h^2 R} \tag{2.113}$$

and $C_h = \frac{1.49}{n} R^{1/6}$ (n = Manning roughness coefficient) in ft-sec units. Equation (2.112) becomes

$$(F_f)_x = \frac{\rho g \, Q|Q|}{A C_h^2 R} \Delta x \tag{2.114}$$

Equations (2.110), (2.111), and (2.114) may be substituted into Equation (2.109) to obtain the expression for $\sum F_x$

$$\sum F_x = - \rho g \frac{\partial h}{\partial x} A \, \Delta x - \frac{\rho g \, Q|Q|}{A C_h^2 R} \Delta x \tag{2.115}$$

It is noted that the integrals in the boundary pressure force Equations (2.110) and (2.111) cancel.

The general one-dimensional momentum equation is obtained by substituting Equation (2.115) into Equation (2.108) and dividing by the product $\rho \, \Delta x$, thus

$$\frac{\partial Q}{\partial t} + U \frac{\partial Q}{\partial x} + Q \frac{\partial U}{\partial x} + g \frac{\partial h}{\partial x} A + g \frac{Q|Q|}{A C_h^2 R} = 0 \tag{2.116}$$

Equation (2.116) together with the continuity equation (2.106) form the pair of equations to be used for the solution of one-dimensional tidal propagation problems in variable area channels.

3.2.3.3 Solution Techniques for Tidal Hydraulic Problems A detailed discussion of solution techniques for tidal hydraulic problems is beyond the scope of this chapter. The emphasis in this section is on citing pertinent references and on considerations which influence the choice of a technique to determine the tidal advective velocity U in the mass transfer Equation (2.95). The choice depends upon the availability and type of field data and upon the desired accuracy. Harleman and Lee (1969) have given a summary and evaluation of one-dimensional solution techniques for estuaries and sea-level canals. The various methods can be grouped in the following categories.

(i) Computation of Tidal Velocity from Simultaneous Solution of the Continuity and Momentum Equations

This method depends upon simultaneous solutions of the continuity and momentum equations. It requires a minimum amount of field data and it is capable of describing nonlinear tidal effects. The continuity and momentum equations can be put into more usable forms by means of the following substitutions. From Figure 2.4

$$h = z_o + d + \eta \tag{2.117}$$

where η is the instantaneous water surface elevation with respect to a reference water level. (η may be positive or negative.) The bottom elevation z_o and the depth d are functions of x but not of time, hence

$$\frac{\partial h}{\partial t} = \frac{\partial \eta}{\partial t} \tag{2.118}$$

and

$$\frac{\partial h}{\partial x} = \frac{\partial z_o}{\partial x} + \frac{\partial d}{\partial x} + \frac{\partial \eta}{\partial x} \tag{2.119}$$

Substituting Equation (2.118) into the continuity equation (2.106) yields

$$b\frac{\partial \eta}{\partial t} + \frac{\partial Q}{\partial x} - q = 0 \tag{2.120}$$

The momentum equation (2.116) contains both the tidal velocity and the discharge; it is convenient to eliminate the velocity in favor of the discharge by the relation $U = Q/A$, to replace $\partial h/\partial x$ by Equation (2.119), and $\partial Q/\partial x$ by Equation (2.120). After dividing each term by the area A , we obtain

$$\frac{1}{A}\frac{\partial Q}{\partial t} + \frac{2Q}{A^2}q - \frac{2bQ}{A^2}\frac{\partial \eta}{\partial t} - \frac{Q^2}{A^3}\frac{\partial A}{\partial x} + g\left[\frac{\partial z_o}{\partial x} + \frac{\partial d}{\partial x} + \frac{\partial \eta}{\partial x}\right] + g\frac{Q|Q|}{A^2{C_h}^2R} = 0 \tag{2.121}$$

The term $\frac{Q^2}{A^3}\frac{\partial A}{\partial x}$ may be shown to be of negligible importance, unless a tidal bore is developed. Equations (2.120) and (2.121) constitute a pair of first-order differential equations in which the water surface elevation η and the tidal discharge Q are the unknowns. The equations are nonlinear and their solution is most readily accomplished by means of finite-difference techniques. Details of such solutions have been provided by several authors including Dronkers (1964 and 1969), Shubinski et al. (1965) who discuss branching estuarial networks, Baltzer and Lai (1968), Balloffet (1969), Liggett and Woolhiser (1967) and Harleman and Lee (1969). These investigations include finite-difference applications of explicit, implicit and characteristics techniques. All such methods require transverse and longitudinal schematization of the estuary into a finite number of segments and the specification of roughness parameters (Chezy or Manning) along the estuary. In addition to specifying the geometry and roughness, two boundary conditions and an initial condition are required. The observed tidal elevations at the ocean entrance of the estuary, i.e., $\eta = f(t)$, almost invariably forms one boundary condition. If the mathematical model spans the entire tidal region, another boundary condition at the landward end is required.

The majority of tidal problems can be grouped into three types according to the physical characteristics of their boundaries and the availability of physical data to be used as an input to the mathematical model.

An Estuary Having a Well-Defined Head of Tide or a Canal Closed at One End. The estuaries in this category are those with a well-defined head of tide such as a fall line or critical flow section. An example is the head of tide at Trenton on the Delaware estuary. The appropriate boundary conditions are

ocean end: $\eta = f(t)$

head of tide or closed end: $Q = 0$

At the ocean end, the ocean tide normally can be obtained from tide tables or from prototype measurements by tide gages. It should be emphasized that the ocean tide need not be sinusoidal; any single tidal cycle record or continuous records may be used. At the head of tide, the condition of no upstream momentum transfer results in the boundary condition $Q = 0$. The freshwater inflow of the river into the last upstream segment of the tidal portion is introduced as a lateral inflow.

An Estuary with an Open End. An open end estuary is one in which the tidal region merges gradually with the upstream river. It is characterized by a progressive reduction of tidal range in the upstream direction. The Savannah estuary is an example of this category. The appropriate boundary conditions are

ocean end: $\eta = f(t)$

open end: $Q = f(t)$

or Q = constant = freshwater discharge of upland river

The ocean end conditions are the same as in the previous section. The open end boundary condition depends on available data. For example, discharge measurements may be available at an upstream location at which the current is always in the ebb direction, however there may be a cyclic variation in the magnitude and $Q = f(t)$ is known. A location farther upstream may be found at which the cyclic variation disappears; in this case the open end boundary condition is Q = constant (equal to the upland river discharge). The location of this point and therefore the length of the segmented tidal channel will change seasonally with variations in the upland discharge. If no measurements are available, it is necessary to assume a length for the tidal channel and to set Q equal to the river discharge. A check on the assumption may be made by determining whether the tidal range at the upstream end becomes small enough to be negligible.

An Estuary Embayment or Canal Connecting Two Bodies of Water. In this category the two bodies of water may be two oceans, as in the case of a sea-level canal, or an ocean and a large lake without tidal fluctuations. An embayment may also be connected to the same ocean through two separate openings. The appropriate boundary conditions are

$$\text{water body (1):} \quad \eta_1 = f_1(t)$$

$$\text{water body (2):} \quad \eta_2 = f_2(t)$$

Other types of boundary conditions may arise in special cases, for example: the specification of discharge at both ends of a channel; the conditions to be applied at a junction of three tidal channels (summation of discharge equal to zero and equal values of η at the junction). The latter is discussed by Dronkers (1964, Chapter X).

As mentioned earlier, it is necessary to assume initial values of η and Q throughout the tidal region in order to begin the numerical solution. Fortunately, as the solution proceeds forward in time, the property of the hyperbolic partial differential equation is such that the effect of the assumed initial condition diminishes rapidly. In the absence of any other information it may be assumed that $\eta = 0$ at $t = 0$ and $Q = 0$ at $t = \Delta t$. Using the known boundary conditions for one tidal cycle, the finite-difference solution proceeds to the end of the first tidal cycle $T + \Delta t$ (where T is the tidal period). The values of η at $t = T$ and Q at $t = T + \Delta t$ become the new initial conditions and the tidal cycle is repeated with the same boundary conditions to the time level $t = 2T + \Delta t$. Thereafter, the computation is repeated to the (k + 1)th tidal cycle. The repeated computation ends when the tidal elevations obtained in the (k + 1)th cycle differ by a small specified amount from those obtained in the (k)th cycle. The solution obtained at the (k + 1)th tidal cycle is referred to as a "quasi-steady state solution." This solution is independent of the magnitudes of the assumed initial conditions. In other words, if the values of η at $t = 0$ and Q at $t = \Delta t$ had been chosen as other than zero, the same quasi-steady solution would have been obtained. The only difference would be in the number of cycles necessary to reach the quasi-steady state. If the assumed values are close to the final values, the number of repeating cycles would be reduced. Mathematically, it is a convergent solution for the given boundary conditions for one tidal cycle.

The Manning coefficient must be specified as a function of x. In an existing estuary or canal, past records of tidal elevation should be used to determine n by matching the computer solution to the field observations. In the case in which no field data is available, n must be assumed on the basis of experience with similar estuaries or canals. Meyers and Schulz (1949) have collected a table of resistance values for some rivers and canals in North America. Dronkers (1964) gives values of the Chezy coefficient for some estuaries in the Netherlands. Baltzer and Lai (1968) have made some detailed computer studies of tidal resistance for short reaches in certain estuaries.

When the computation yielding $\eta = f(x,t)$ and $Q = f(x,t)$ has been completed for the tidal region, any available field data for tidal amplitude and phase can be used to check the geometric schematization and assumed roughness. If appreciable differences occur, the roughness magnitude and its spatial variation can be adjusted until agreement is obtained. This approach is particularly useful in the prediction of the effect of proposed geometric changes, such as dredging, on tidal motion in estuaries. The tidal discharge Q (or velocity U) obtained in this manner is a direct input in the advective term of the mass transfer equation (2.95). The following figures taken from Harleman and Lee (1969) illustrate the results of a finite-difference, digital computer calculation of tidal motion in the Delaware estuary. Figure 2.5 shows a comparison of the computed and observed mean tidal range along the Delaware from Miah Maull (in Delaware Bay) to Trenton (the head of tide for this closed-end estuary). Figure 2.6 shows an important feature of the nonlinear solution. The observed and computed tidal elevations versus time are plotted at Miah Maull, a middle section and at the Trenton end of the estuary. The progressive distortion of the tide curve from a sinusoidal shape in Delaware Bay to a highly nonsinusoidal curve at Trenton is clearly indicated. The computed values of the maximum flood and ebb velocities are plotted as a function of distance along the estuary in Figure 2.7. The corresponding maximum discharges are given in Figure 2.8 for fresh water inflow of 11,650 cfs at Trenton. Figure 2.9 shows the time variation of the tidal velocity and discharge at two sections through one tidal period. Again, the nonlinear tidal advection effects are shown by the nonsinusoidal shape of the velocity curve and by the fact that the duration of flood velocity is 5.2 hours, whereas the duration of the ebb velocity is 7.2 hours at a section 58 miles from Mich Maull.

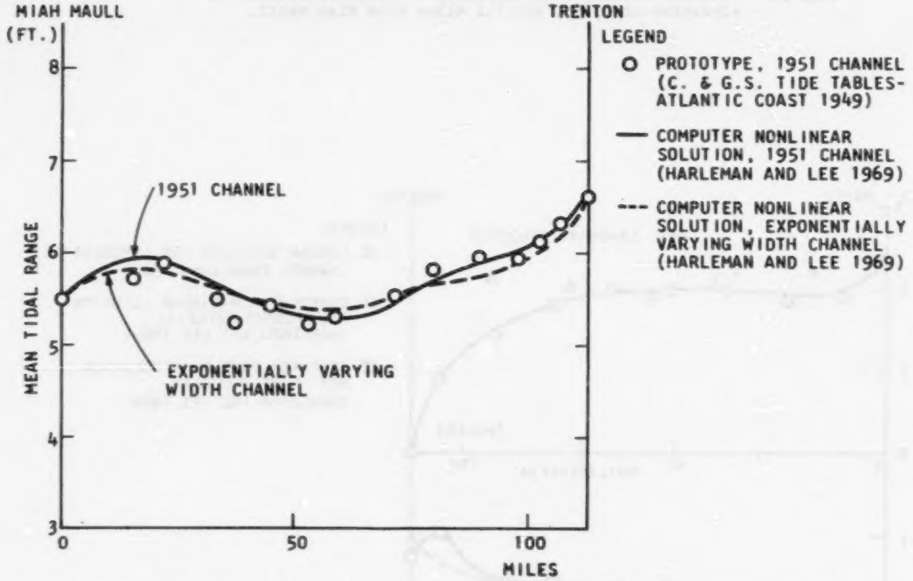


Fig. 2.5 Delaware Estuary -- mean tidal range.

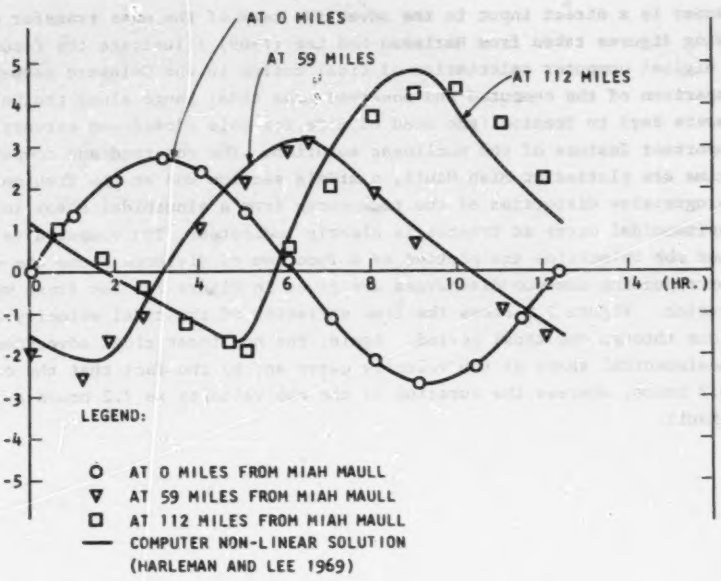


Fig. 2.6 Delaware Estuary (1951 Channel) -- Tidal variations in elevation at 0, 59, and 112 miles from Miah Maull.

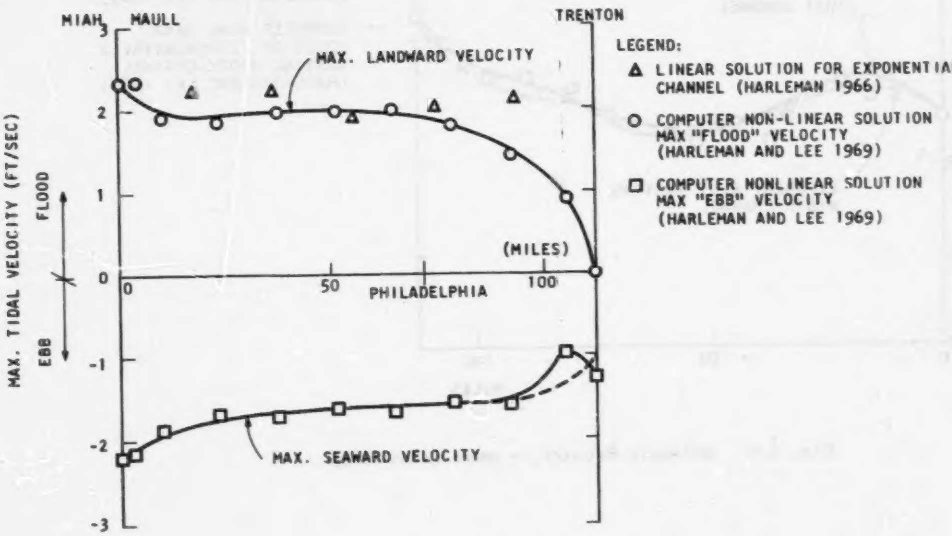


Fig. 2.7 Delaware Estuary (1951 Channel) -- Maximum tidal velocities.

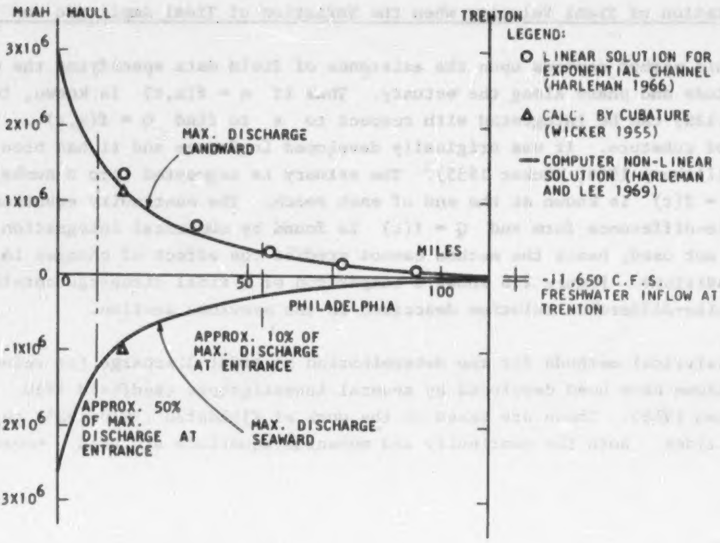


Fig. 2.8 Delaware Estuary (1951 Channel) -- Maximum tidal discharges.

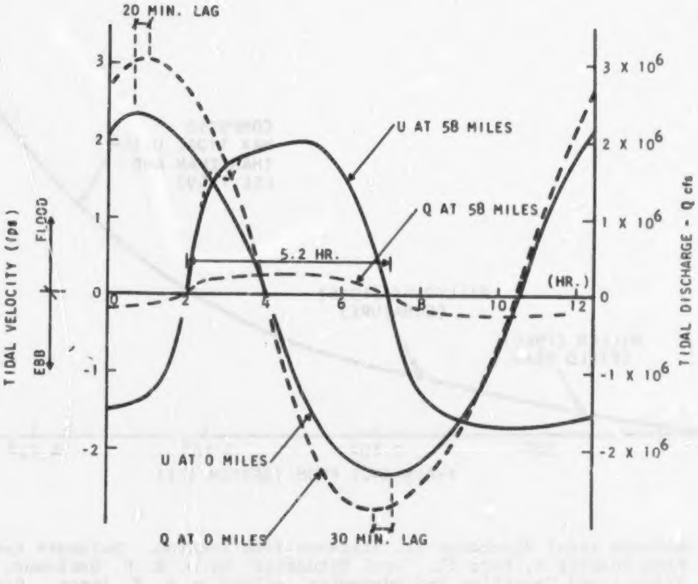


Fig. 2.9 Delaware Estuary (1951 Channel) -- Tidal velocities and discharges at 0 and 58 miles from Miah Maull. Harleman and Lee (1969).

(ii) Computation of Tidal Velocity when the Variation of Tidal Amplitude and Phase are Known

This method depends upon the existence of field data specifying the distribution of tidal amplitude and phase along the estuary. Thus if $\eta = f(x,t)$ is known, the continuity equation (2.120) can be integrated with respect to x to find $Q = f(x,t)$. This is known as the method of cubature. It was originally developed in France and it has been applied to the Delaware (Pillsbury 1956, Wicker 1955). The estuary is segmented into a number of finite reaches in which $h = f(t)$ is known at the end of each reach. The continuity equation (2.120) is written in finite-difference form and $Q = f(t)$ is found by numerical integration. The momentum equation is not used, hence the method cannot predict the effect of changes in estuary geometry or other conditions. Figure 2.8 shows a comparison of a tidal discharge obtained by cubature with the finite-difference solution described in the previous section.

Analytical methods for the determination of tidal discharge (or velocity) when $\eta = f(x,t)$ is known have been developed by several investigators (Redfield 1950, Ippen and Harleman 1958, Harleman 1966). These are based on the work of Fjeldstad (1918-1925) on damped, co-oscillating tides. Both the continuity and momentum equations are used. However, the quadratic

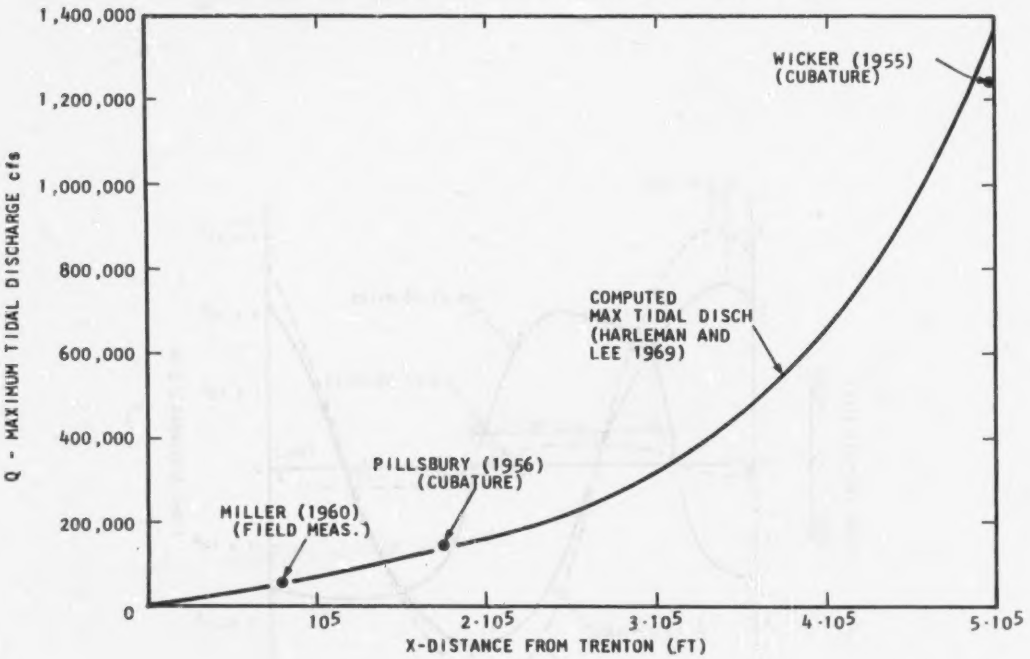


Fig. 2.10 Maximum tidal discharge vs. distance from Trenton. Delaware Estuary. From Chapter X, Part II, "Real Estuaries" by D. R. F. Harleman, in Estuary and Coastline Hydrodynamics, edited by A. T. Ippen. Copyright 1966 by McGraw-Hill, Inc. Used with permission of McGraw-Hill Book Company.

frictional term in the latter is replaced by a linear term. In addition, it is assumed that the tidal motion is harmonic throughout the tidal portion. The problem of specifying the estuary roughness is avoided by making use of the field data on tidal amplitude and phase throughout the estuary. A comparison of the maximum tidal discharges in the Delaware computed by the method of cubature and damped co-oscillating tide is shown in Figure 2.10 (Harleman 1966). It should be emphasized that if the tidal velocity is assumed to be harmonic, the non-tidal advective velocity due to freshwater inflow must be added as a separate term. Otherwise the flushing effect of the upland discharge would be lost. This is discussed in the following section.

(iii) Direct Measurement of Tidal Velocities

There are probably few cases where sufficient field measurements in estuaries are available to determine $U = f(x,t)$ directly. In situations where observations of maximum tidal velocities can be made at certain sections, it may be sufficient, as a first approximation, to utilize an ad hoc equation of the form

$$U = U_f(x) + U_T(x) \sin \left[\sigma t - F(x) \right] \tag{2.122}$$

where U_f is the velocity due to non-tidal (freshwater) inflow, U_T is the maximum tidal velocity, $\sigma = 2\pi/T$ (T = tidal period) and $F(x)$ is a function describing the change in the phase of tidal velocities along the estuary. Equation (2.122) is the simplest representation of the advective velocity term in the mass transfer equation (2.95) in real time.

3.2.4 Longitudinal Dispersion in the Real Time Mass Transfer Equation

The objective of this section is to summarize various methods of determining longitudinal dispersion coefficients. The first approach is an analytical one considering the fluid mechanics of dispersion in an oscillating flow. The second is an empirical one in which the dispersion coefficient is determined by comparing a solution of the mass transfer equation with the measured concentration distribution of some substance in an estuary. The same dispersion coefficient is then used to predict the concentration distribution of some other substance. In practice, the empirical determination of dispersion coefficients is limited by the requirement that all source and sink (decay) terms for the substance must be known with reasonable accuracy. Therefore, the second method is restricted to naturally conservative substances such as salinity or to artificially introduced tracers for which decay and absorption rates can be determined. In the past, observational data from either the prototype or a hydraulic model have been used in the empirical method. Chapter V includes a discussion of certain difficulties in the determination of dispersion coefficients from observations in distorted hydraulic models.

A physical understanding of longitudinal dispersion can be gained by considering a steady, uniform, turbulent flow in a pipe. Assume that a finite amount of a tracer substance is injected instantaneously and uniformly across the entire flow section. Because of the velocity distribution the tracer near the center of the pipe moves downstream much faster than the tracer near the walls. Lateral turbulent mixing maintains uniform concentrations at various sections; however, there is a large longitudinal spreading due to the relative velocity between adjacent layers. After a certain time, the longitudinal distribution of concentration of the tracer approaches a Gaussian distribution about the peak. The advective term in the one-dimensional mass transfer equation contains the average longitudinal velocity at the section and it is therefore unable to account for the longitudinal spreading due to the velocity dis-

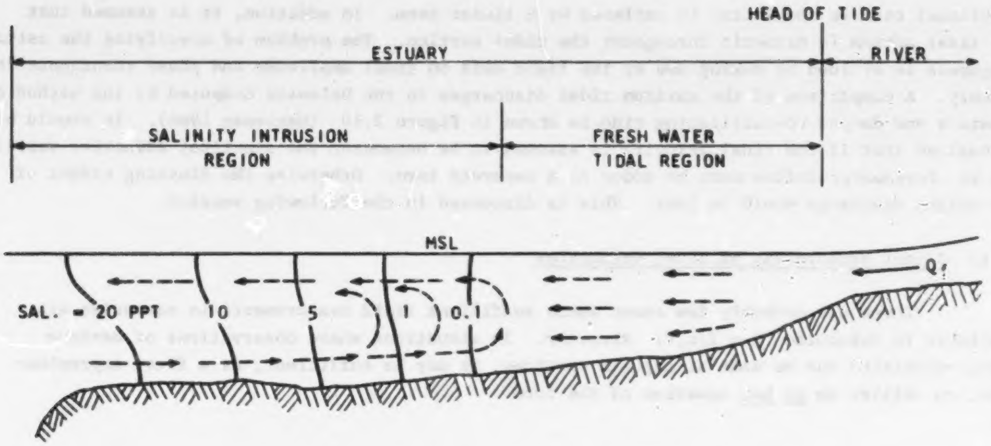


Fig. 2.11 Mean current and salinity distribution in a mixed estuary.

tribution. The mass transfer due to the velocity distribution is combined with that due to turbulent diffusion and the total effect is represented by a longitudinal dispersion coefficient. Qualitatively, the more non-uniform the velocity distribution, the larger the dispersion coefficient. On this basis we should expect to find much larger dispersion coefficients within the salinity intrusion portions of estuaries in comparison with the non-saline tidal regions. It is well known that in the salinity intrusion region the tidal velocities are modified by the gravitational circulation set up by the longitudinal density gradients. A typical estuary can be divided into a salinity intrusion region and a fresh water tidal region as shown in Figure 2.11. The line of demarcation is not fixed since the longitudinal extent of salinity intrusion varies during a tidal period by a distance equal to the tidal excursion. In addition, the intrusion distance depends on the magnitude of the fresh water inflow into the estuary.

At the present there is no analytical method of predicting longitudinal dispersion coefficients within the salinity intrusion region of an estuary. We must therefore rely on empirical determinations based on observed salinity distributions. Fortunately, salinity is relatively easy to measure and it usually may be considered a conservative substance. The empirical determination of longitudinal dispersion coefficients in the fresh water tidal region is much more difficult because of the absence of any natural, conservative substance. Field tests, involving the injection of artificial tracers and subsequent measurement of time and space concentrations are difficult, time consuming and expensive. Fortunately, considerable progress has been made analytically and it now appears possible to predict longitudinal dispersion coefficients in tidal regions containing water of uniform density, with an accuracy sufficient for practical purposes. It should be noted that a tidal region containing water of uniform salinity can be considered in the same category as a freshwater tidal region. A quantitative discussion of longitudinal dispersion in the uniform density and salinity intrusion regions is given in the following sections.

3.2.4.1 Longitudinal Dispersion Coefficient in Regions of Uniform Density

(i) Dispersion in Steady, Unidirectional Flow. Taylor (1954) appears to have been the first to determine a numerical value for the longitudinal dispersion coefficient E_L. He considered steady, uniform, axisymmetrical turbulent flow in a long, straight pipe and assumed that the concentration c at any point in the pipe could be written as $(c_x + c_r)$ where c_x was a function of x only and c_r was a function of the radial coordinate r only. He assumed the form of the radial velocity distribution. The turbulent (mass) diffusivity was assumed to be isotropic and equal to the eddy viscosity. Considering the asymptotic solution to the axisymmetric mass balance equation, Taylor determined that the dimensionless longitudinal dispersion coefficient for a pipe should be

$$E_L = 10.1\, r_o u_* \qquad (2.123)$$

where r_o is the pipe radius and $u_* = \sqrt{\tau_o/\rho}$ is the shear velocity (τ_o is the shear stress at the wall).

Elder (1959) carried out a computation similar to Taylor's for a steady, uniform, two-dimensional, infinitely wide open channel flow with a logarithmic velocity distribution in the vertical direction. Elder's result is

$$E_L = 5.9\, d\, u_* = 5.9\, d \sqrt{gDS_E} \qquad (2.124)$$

where d is the depth of flow. The predicted longitudinal dispersion coefficients given by Equations (2.123) and (2.124) have been confirmed experimentally by injecting tracers into turbulent flow in uniform pipes and wide open channels.

Taylor's equation (2.123) can be rewritten in terms of the channel flow and resistance parameters by noting that

$$u_* = \frac{\sqrt{f}}{\sqrt{8}}\, U$$

where f is the pipe friction factor and U is the average velocity. The Chezy coefficient relates f to the Manning roughness n and the hydraulic radius R_h,

$$C_h = \frac{\sqrt{8g}}{\sqrt{f}} = \frac{1.49}{n} R_h^{1/6}$$

Thus, replacing r_o by $2R_h$ for a pipe, Equation (2.123) becomes

$$E_L = 77\, n\, U\, R_h^{5/6} \text{ (in ft-sec units)} \qquad (2.125)$$

Fischer (1967 and 1968) analyzed concentration distributions produced by tracers introduced into non-tidal rivers and concluded that Equation (2.125) predicts longitudinal dispersion coefficients which are too small, in some cases by two orders of magnitude. He attributes this to the fact that longitudinal dispersion in rivers is produced primarily by velocity variations in the lateral direction rather than by velocity variations in the vertical direction.

(ii) Dispersion in an Oscillating Flow. Holley et al. (1970) and Fischer (1969) have investigated the implications of the above conclusions with regard to dispersion associated with tidal motion in constant density regions of estuaries. They have shown that dispersion in an oscillating flow depends on the ratio of the period of oscillation (T) to a time scale for cross-sectional mixing τ_o . Because estuaries are relatively wide and shallow, two cross-sectional mixing time scales can be defined: one for transverse mixing and one for vertical mixing. Using values typical of the upper Delaware estuary, it is estimated that the time scale for transverse mixing is approximately 200 times longer than the tidal period. On the other hand, the time scale for vertical mixing is approximately 15 times shorter than the tidal period. On this basis, velocity variations in the lateral direction would contribute very little to the longitudinal dispersion and it is concluded that the velocity distribution in the vertical direction is of primary importance. Therefore, the open channel modification of Taylor's equation (2.125) would be appropriate in most estuaries.

The remaining question is the velocity which should be used in the modified Taylor equation when it is applied to an oscillating rather than a unidirectional flow. If the absolute value of the tidal velocity were used, E_L would vary with time throughout the tidal cycle with two peaks as shown in Figure 2.12. Holley and Harleman (1965, see also Harleman et al. 1966) conducted dispersion experiments in a longitudinal oscillating flow and concluded that the dispersion coefficient could be assumed to be constant throughout a tidal cycle if the time average of the absolute value of the tidal velocity were used in the Taylor equation. If the temporal variation of the tidal velocity is approximately sinusoidal, the time average of the absolute value is $2/\pi$ times the maximum tidal velocity U_{max} . In an estuary it is expected that bends and channel irregularities will cause an increase in the longitudinal dispersion in comparison with a straight channel. On this basis it is suggested that the modified Taylor equation (2.125) be increased by a factor of 2 ; the proposed equation, in terms of the maximum tidal velocity, is

$$E_L = 100\ n\ U_{max}\ R_h^{5/6} \text{ (in ft-sec units)} \qquad (2.126)$$

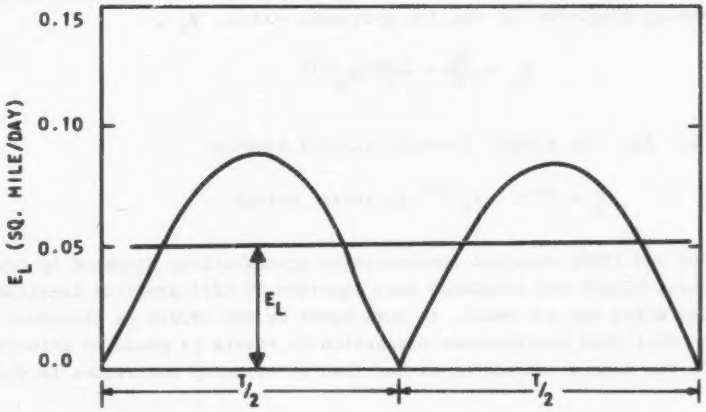


Fig. 2.12 Variation of longitudinal dispersion coefficient in a tidal period.

The longitudinal dispersion coefficient is frequently expressed in square miles per day rather than in square feet per second. (1 sq. mile/day = 320 ft^2/sec.) Thus Equation (2.126) can be written in mixed units as

$$E_L = 0.3\, n\, U_{max}\, R_h^{5/6} \begin{bmatrix} E_L \text{ in sq mi/day} \\ U_{max} \text{ and } R_h \text{ in ft-sec} \end{bmatrix} \qquad (2.127)$$

In the freshwater, tidal portion of the Delaware near Philadelphia the following values are appropriate (Harleman and Lee 1969):

Manning roughness, $n = 0.028$
maximum tidal velocity, $U_{max} = 2.0$ ft/sec
hydraulic radius, $R_h = 20$ ft

The order of magnitude of the longitudinal dispersion coefficient near Philadelphia, given by Equations (2.126) and (2.127), is $E_L = 70$ ft^2/sec or 0.2 sq mi/day .

The validity of the modified Taylor equation for the longitudinal dispersion coefficient in a constant density tidal region can be tested by comparing the predicted value with a dispersion coefficient determined from a field test. The necessary prototype measurements are very expensive and time consuming, and only a few such tests have been conducted. Hetling and O'Connell (1966) have reported the results of a dye dispersion test in the freshwater tidal portion of the Potomac. Rhodamine dye was discharged continuously for a period of 13 days at a point below Washington. Dye concentration observations were made throughout the upper 25 miles of the estuary for a period of 34 days following the release. The observed value of E_L in the vicinity of the release point was reported to be 0.2 sq mi/day. Using the following geometric and tidal quantities assumed to be characteristic of this reach of the Potomac:

$$n = 0.035$$
$$U_{max} = 1.6 \text{ ft/sec}$$
$$R_h = 13 \text{ ft}$$

the calculated value from the modified Taylor equation (2.127) is $E_L = 0.14$ sq mi/day which is in good agreement with the reported value.

3.2.4.2 Longitudinal Dispersion in Salinity Intrusion Regions Longitudinal dispersion is a result of spatial variations in the longitudinal tidal velocities at a section. In the constant density tidal region the velocity distribution is due to frictional shear exerted at the section boundary. In the region of salinity intrusion, the longitudinal density gradients associated with the transition from ocean water to fresh water cause significant changes to the boundary shear velocity distribution. This is due to the superposition of the frictional effect and a large-scale density-driven horizontal circulation in which near-bottom velocities are augmented during the flood phase of the tide and retarded during the ebb phase. The salinity circulation is shown schematically in Figure 2.13. A set of tidal velocity observations (as a function of depth) at ten percent intervals throughout a tidal period is shown in Figure 2.14. The data was taken in the salinity intrusion flume at the Waterways Experiment Station (Harleman and Ippen 1967 and 1969) at a station within the salinity intrusion region. The fact that the ebb velocity distributions are much more nonuniform than the flood velocity distributions is evident.

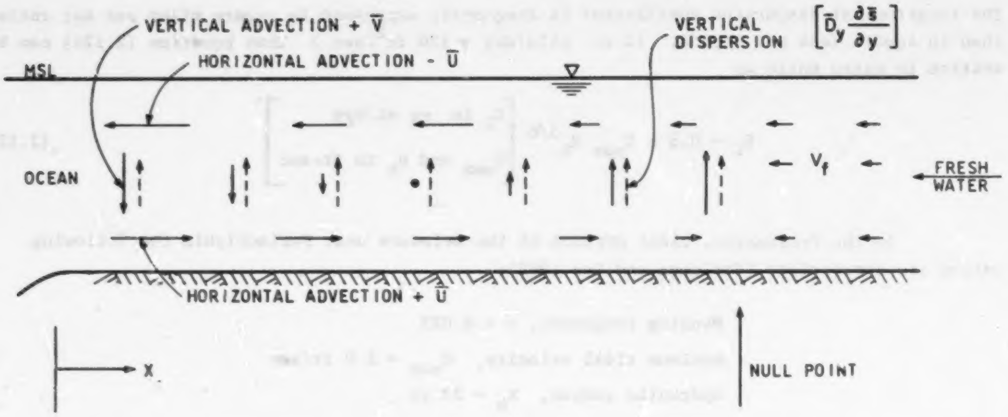

VERTICAL ADVECTION + $\bar{V}$
HORIZONTAL ADVECTION - $\bar{U}$
VERTICAL DISPERSION
$\left[\bar{D}_y \frac{\partial \bar{s}}{\partial y}\right]$
MSL
OCEAN
V_f
FRESH WATER
HORIZONTAL ADVECTION + $\hat{U}$
X
NULL POINT

Fig. 2.13 Schematic diagram of estuary salinity circulation.

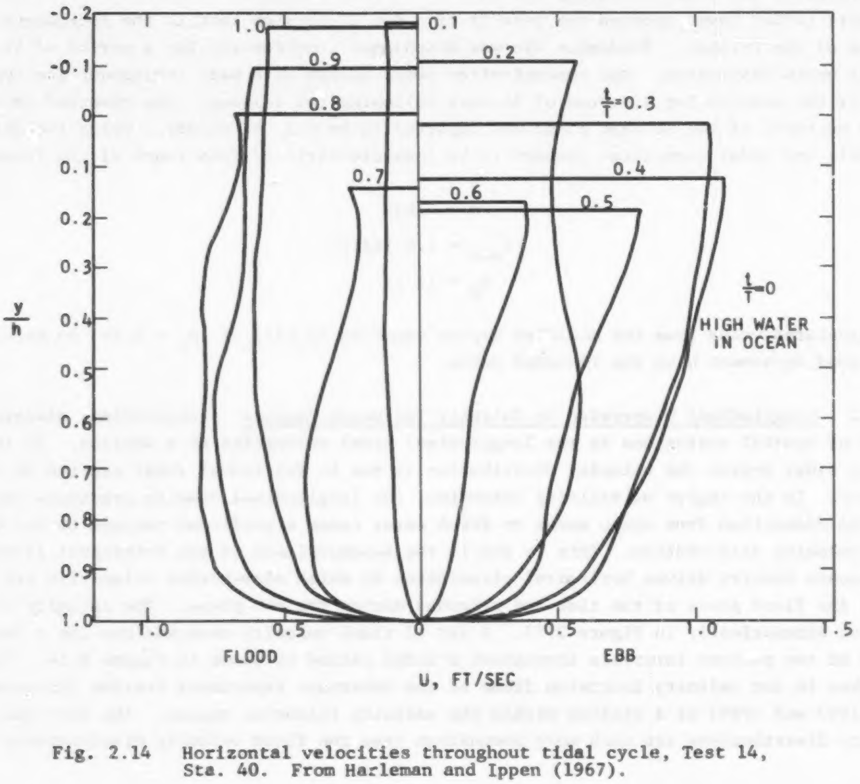


Fig. 2.14 Horizontal velocities throughout tidal cycle, Test 14, Sta. 40. From Harleman and Ippen (1967).

The distortion of velocity distribution by the salinity intrusion is even more apparent when the velocity distributions are averaged over a tidal period. A set of such velocity distributions at various distances from the ocean entrance is shown in Figure 2.15. The time-average tidal velocity at each depth is normalized by dividing by the magnitude of the freshwater velocity. The upstream limit of salinity intrusion clearly lies between stations 160 and 200.

The longitudinal dispersion coefficient in the salinity intrusion region will be designated by E_L' in order to distinguish it from the dispersion coefficient in the constant density tidal region.

The physical interrelationships between the tidal motion and salinity intrusion can be demonstrated by means of field and laboratory observations in estuaries of uniform geometry. We consider the situation in real tidal time by coupling the one-dimensional equations of continuity, momentum and the mass transfer equation for salt.

If the width b is constant and z_o (Figure 2.4) is zero, the instantaneous depth is h. Thus the cross-sectional area is $A = bh$ and the tidal discharge is given by $Q = bhU$. The continuity equation (2.106) becomes

$$\frac{\partial h}{\partial t} + U\frac{\partial h}{\partial x} + h\frac{\partial U}{\partial x} = 0 \qquad (2.128)$$

where the lateral inflow q is also assumed to be negligible. Substituting Equation (2.128) into Equation (2.116), the momentum equation becomes

$$\frac{\partial U}{\partial t} + U\frac{\partial U}{\partial x} + g\frac{\partial h}{\partial x} + g\frac{U|U|}{C_h^2 R} = 0 \qquad (2.129)$$

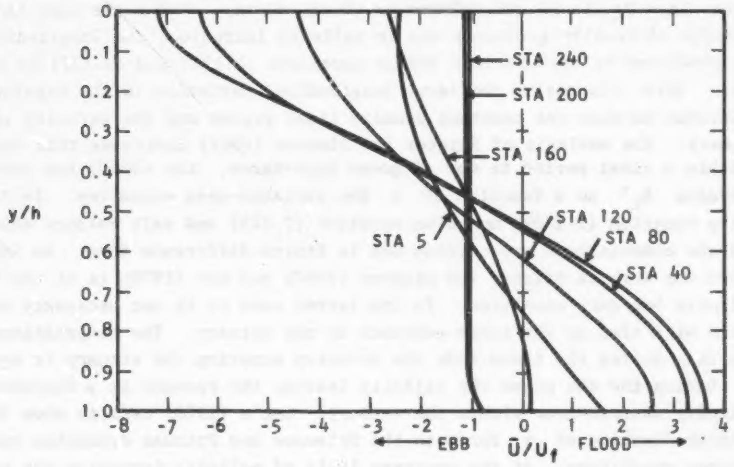


Fig. 2.15 Vertical variation of time-averaged tidal velocity relative to freshwater velocity: Test No. 16. Harleman and Ippen (1967).

In a similar manner, the mass transfer equation can be simplified for an estuary of uniform width. By expanding the derivatives and making use of the continuity equation (2.128) the mass transfer equation (2.95) for salt (a conservative substance for which r_i and r_e are zero) can be written as

$$\frac{\partial C}{\partial t} + U \frac{\partial C}{\partial x} = \frac{1}{h} \frac{\partial}{\partial x} \left(h \, E_L' \, \frac{\partial C}{\partial x} \right) \tag{2.130}$$

The three equations can be solved for the three unknowns, $h = f(x,t)$, $U = f(x,t)$ and $C = f(x,t)$ provided that the proper initial and boundary conditions are given. In addition, the roughness (Chezy or Manning) and the longitudinal dispersion coefficient E_L' must be specified as functions of x and t.

Stigter and Siemons (1967) have carried out a finite-difference solution using an implicit scheme. The boundary and initial conditions for the tidal calculations have already been discussed in Section 3.2.3.3. The observed salinity variation with time at the ocean entrance of the estuary was used as the salinity boundary condition. Both C_h and E_L' were assumed to be constant in time and the roughness C_h was also assumed to be constant with respect to x. The value of C_h chosen was the one giving the best agreement between the calculated and observed tidal elevations. The dispersion coefficient $E_L' = f(x)$ was adjusted until a best fit was obtained between the calculated and observed salinity concentrations. The results are shown in Figure 2.16 for both the temporal and spatial distribution of salinity. The observed salinities are field measurements from the Rotterdam Waterway. This is a tidal estuary of almost uniform depth and width, carrying a portion of the freshwater discharge of the Rhine, and joining the North Sea at Hook of Holland. The longitudinal dispersion coefficient was determined to be a function of x of the form

$$E_L' = 13{,}000 \left(1 - \frac{x}{L}\right)^3 , \ (\text{ft}^2/\text{sec}) \tag{2.131}$$

where L is the length of the entire tidal region of the estuary. The magnitude of E_L' at the ocean entrance $(x = 0)$ is 13,000 ft^2/sec or 40 sq mi/day. Under the same tidal conditions, in the absence of density gradients due to salinity intrusion, the longitudinal dispersion coefficient predicted by the modified Taylor equations (2.126) and (2.127) is 175 ft^2/sec or 0.5 sq mi/day. This illustrates the large longitudinal variation in the magnitude of the dispersion coefficient between the constant density tidal region and the salinity intrusion region of an estuary. The analysis of Stigter and Siemons (1967) indicates that the time variation of E_L' within a tidal period is not of great importance. Lee (1970) has used a similar approach to determine E_L' as a function of x for variable-area estuaries. In this case the general continuity equation (2.120), momentum equation (2.121) and salt balance equation (2.95) must be used and the computations are carried out in finite-difference form. An important difference between the work of Stigter and Siemons (1967) and Lee (1970) is in the treatment of the ocean salinity boundary condition. In the latter case it is not necessary to know the salinity variation with time at the ocean entrance to the estuary. The computational program is arranged such that during the flood tide the salinity entering the estuary is equal to the ocean salinity. During the ebb phase the salinity leaving the estuary is a function of the longitudinal salinity distribution within the estuary. Lee's (1970) results show that E_L' is essentially a linear function of x for both the Delaware and Potomac estuaries under various freshwater discharge conditions. At the upstream limit of salinity intrusion the value of E_L' approaches the Taylor value appropriate to the nonsaline region (see Equation 2.126). The maximum value of E_L' is reached near the ocean entrance.

The analyses presented above are examples of methods of determining the longitudinal dispersion coefficient as a function of x from salinity observations during one tidal period.

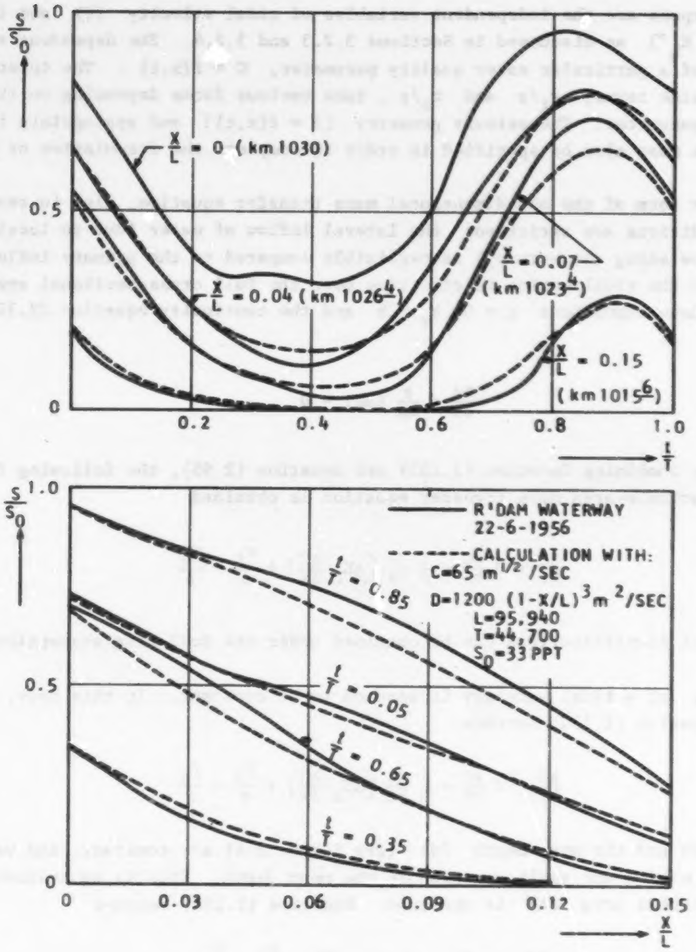


Fig. 2.16 Comparison of calculated and observed temporal and spatial salinity distributions in the Rotterdam Waterway. Stigter and Siemons (1967).

3.2.5 Discussion of the Real Time Mass Transfer Equation

The foregoing developments have been primarily concerned with the hydrodynamic aspects of one-dimensional mathematical models for estuarine water quality control. The central relationship is the mass transfer Equation (2.95) in which the real time variables are related to the tidal motion.

$$\frac{1}{A}\frac{\partial}{\partial t}(AC) + \frac{1}{A}\frac{\partial}{\partial x}(AUC) = \frac{1}{A}\frac{\partial}{\partial x}\left(AE_L\frac{\partial C}{\partial x}\right) + \frac{r_i}{\rho} + \frac{r_e}{\rho} \qquad (2.95)$$

The hydrodynamic inputs are the independent variables of tidal velocity (U) and longitudinal dispersion (E_L or E_L') as discussed in Sections 3.2.3 and 3.2.4. The dependent variable is the concentration of a particular water quality parameter, $C = f(x,t)$. The internal and external source and sink terms, r_i/ρ and r_e/ρ , take various forms depending on the nature of the water quality parameter. The estuary geometry $[A = f(x,t)]$ and appropriate initial and boundary conditions must also be specified in order to complete the formulation of the problem.

A simpler form of the one-dimensional mass transfer equation, also in real time, can be used if two conditions are satisfied: the lateral inflow of water (due to local tributaries or subsurface inflow along the estuary) is negligible compared to the primary inflow at the head of the estuary, and the tidal motion is effective over the full cross-sectional area at all sections. Under these conditions $q = 0$, $b_s = b$ and the continuity equation (2.105) can be written as

$$\frac{\partial A}{\partial t} + \frac{\partial}{\partial x}(AU) = 0 \tag{2.132}$$

since $Q = AU$. By combining Equation (2.132) and Equation (2.95), the following form of the one-dimensional, variable-area mass transfer equation is obtained

$$\frac{\partial C}{\partial t} + U\frac{\partial C}{\partial x} = \frac{1}{A}\frac{\partial}{\partial x}\left(AE_L\frac{\partial C}{\partial x}\right) + \frac{r_i}{\rho} + \frac{r_e}{\rho} \tag{2.133}$$

Additional simplifications can be obtained under the following assumptions:

(i) The width (b) of a tidal waterway is assumed to be constant. In this case, the depth $h = f(x,t)$ and Equation (2.133) becomes

$$\frac{\partial C}{\partial t} + U\frac{\partial C}{\partial x} = \frac{1}{h}\frac{\partial}{\partial x}\left(hE_L\frac{\partial C}{\partial x}\right) + \frac{r_i}{\rho} + \frac{r_e}{\rho} \tag{2.134}$$

(ii) Both the width and the mean depth (d) (see Figure 2.4) are constant, and variations in depth due to tidal motion are small compared to the mean depth. This is equivalent to assuming that the cross-sectional area (A) is constant. Equation (2.133) becomes

$$\frac{\partial C}{\partial t} + U\frac{\partial C}{\partial x} = \frac{\partial}{\partial x}\left(E_L\frac{\partial C}{\partial x}\right) + \frac{r_i}{\rho} + \frac{r_e}{\rho} \tag{2.135}$$

(iii) The cross-sectional area is assumed to be constant and the longitudinal dispersion coefficient is assumed to be independent of x . This approximation may be reasonable in the constant density portion of certain estuaries in which the magnitude of the tidal velocity at a given time is essentially independent of x . In this case Equation (2.133) becomes

$$\frac{\partial C}{\partial t} + U\frac{\partial C}{\partial x} = E_L\frac{\partial^2 C}{\partial x^2} + \frac{r_i}{\rho} + \frac{r_e}{\rho} \tag{2.136}$$

In all of the approximate forms of Equation (2.95), Equations (2.133) - (2.136), U represents the tidal velocity which, in general, is a function of x and t . Certain physical properties of the real time mass transfer equations are demonstrated in the following sections.

3.2.6 Solution of the Real Time Mass Transfer Equation in a Uniform Estuary

Analytical solutions of the real time mass transfer equation for estuaries of simple geometry are useful: (i) in providing a graphical visualization of the advection and dispersion processes in tidal motion; (ii) as a basis of comparison with mathematical models involving longer periods of time averaging; (iii) as a basis for determining the accuracy of finite-difference formulations.

The essential features of the real time solution can be demonstrated by considering an idealized estuary of constant cross-sectional area; the tidal velocity is a function of time and independent of x and the longitudinal dispersion coefficient is constant. The concentration distribution due to the introduction of a substance at a certain section is to be determined as a function of x and t. The substance is non-conservative and undergoes internal decay in accordance with a first-order reaction given by Equation (2.97). There are no external sources or sinks other than at the section of injection. Under these conditions the general mass transfer equation (2.95) reduces to the form of Equation (2.136),

$$\frac{\partial C}{\partial t} + U \frac{\partial C}{\partial x} = E_L \frac{\partial^2 C}{\partial x^2} - K_d C \tag{2.137}$$

where $U = f(t)$ and E_L and K_d are constants.

Initially it is desired to find the solution of Equation (2.137) in an infinite channel for an instantaneous release of W pounds of pollutant at $x = 0$ at time $t = \tau$. The analytical solution can be obtained by introducing the following changes of variables. Let ζ be a new concentration variable such that

$$C = \zeta e^{-K_d(t - \tau)} \tag{2.138}$$

Let χ be a new longitudinal coordinate distance measured with respect to a cross-sectional plane moving with the velocity $U(t)$. Therefore

$$x = \chi + \int_\tau^t U(t)\, dt \tag{2.139}$$

Introducing the above into Equation (2.137), the mass transfer equation can be written as

$$\frac{\partial \zeta}{\partial t} = E_L \frac{\partial^2 \zeta}{\partial \chi^2} \tag{2.140}$$

which is the elementary form of the diffusion equation known as Fick's second law. The solution for an instantaneous release (delta function) is

$$\zeta = \frac{W}{\gamma A \sqrt{4\pi E_L (t-\tau)}} \exp\left[-\frac{\chi^2}{4E_L(t-\tau)}\right] \tag{2.141}$$

where γ is the specific weight of the receiving fluid. Equation (2.141) can be written in terms of the original concentration variable by substituting Equation (2.138), therefore

$$C = \frac{W}{\gamma A \sqrt{4\pi E_L (t-\tau)}} \exp\left[-\frac{\chi^2}{4E_L(t-\tau)} - K_d(t-\tau)\right] \tag{2.142}$$

The solution for a continuous input of pollutant at a rate w (pounds per second) can be obtained from Equation (2.142) by considering the continuous release to be made up of a continuous series of incremental instantaneous releases of magnitude dW where

$$dW = w\,d\tau \tag{2.143}$$

The increment of concentration resulting from each increment of instantaneous release is given by Equation (2.142) with C replaced by dC and W by dW. Integrating Equation (2.142) with respect to τ sums the effect of the continuous series of instantaneous releases. The concentration distribution at time t for a continuous release beginning at $t = 0$ is given by

$$C = \int_0^t \frac{w}{\gamma A\sqrt{4\pi E_L(t-\tau)}} \exp\left[-\frac{\chi^2}{4E_L(t-\tau)} - K_d(t-\tau)\right] d\tau \tag{2.144}$$

Finally, it is desirable to return to the original variable x in place of χ by means of Equation (2.139). This requires the specification of $U(t)$. We can, without loss of generality, demonstrate the essential features of the real time model by assuming that the tidal velocity is a harmonic function of time of the form

$$U(t) = U_f + U_T \sin \sigma t \tag{2.145}$$

Equation (2.145) is a special case of Equation (2.122) in which U_f, the velocity due to freshwater inflow, and U_T, the amplitude of the oscillating component of the velocity, are constants. In addition, the phase lag $F(x) = 0$ and $\sigma = 2\pi/T$ (T = tidal period). Substituting Equation (2.145) in Equation (2.139) and eliminating χ in Equation (2.144), we have

$$C = \int_0^t \frac{w}{\gamma A\sqrt{4\pi E_L(t-\tau)}} \exp\left\{-\frac{\left[x - U_f(t-\tau) + \frac{U_T}{\sigma}(\cos \sigma t - \cos \sigma\tau)\right]^2}{4E_L(t-\tau)} - K_d(t-\tau)\right\} d\tau \tag{2.146}$$

If the injection rate w is a constant, Equation (2.146) can be written in dimensionless form by defining a reference concentration

$$C_o = \frac{w}{\gamma A U_f} \tag{2.147}$$

Therefore,

$$\frac{C}{C_o} = \int_0^t \frac{U_f}{\sqrt{4\pi E_L(t-\tau)}} \exp\left\{-\frac{\left[x - U_f(t-\tau) + \frac{U_T}{\sigma}(\cos \sigma t - \cos \sigma\tau)\right]^2}{4E_L(t-\tau)} - K_d(t-\tau)\right\} d\tau \tag{2.148}$$

The integral of Equation (2.148) cannot be evaluated analytically; however, it can be programmed readily for numerical evaluation on a computer.

Calculated concentration distributions for a continuous injection, as given by Equation (2.148), are shown by the curves in Figure 2.17 for a conservative substance in which $K_d = 0$. The dimensionless concentration C/C_o is plotted as a function of the dimensionless longitudinal distance x/λ, where λ is the tidal excursion. The tidal excursion is the distance traveled by a particle of water in half the tidal period. For the tidal velocity given by Equation (2.145)

$$\lambda = \frac{U_T T}{\pi} \tag{2.149}$$

Concentration distributions at four different times are shown in terms of a dimensionless time variable

$$N = t/T \tag{2.150}$$

where N is the number of tidal periods from the beginning of injection at $x = 0$ and $t = 0$. Values of N equal to an integer correspond to times of high water slack (i.e., $N = 30$ and 400) and the half-integer values (i.e., $N = 30.5$ and 400.5) to times of low water slack. Within each tidal period, the pollutant is advected upstream and downstream of the injection section at $x = 0$, and the concentration increases slowly until a quasi-steady state is reached at about 400 tidal periods.

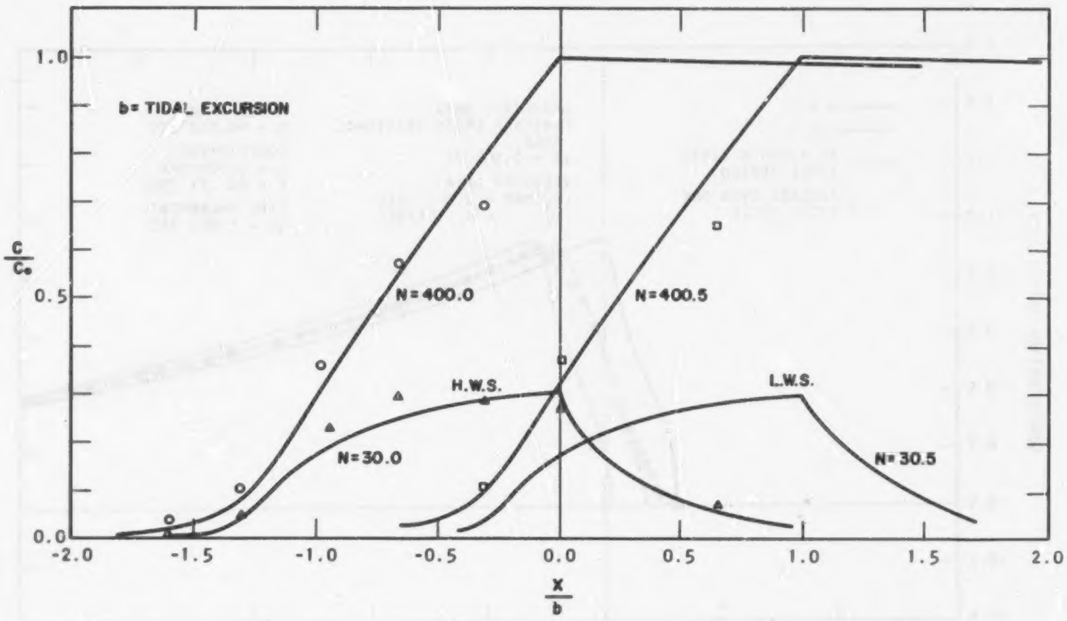


Fig. 2.17 Continuous injection dispersion test showing comparison of data with Equation (2.148).

Laboratory experiments conducted by Harleman et al. (1966) in a uniform, oscillating flow system indicate good agreement with the theoretical curves. The longitudinal dispersion coefficient was calculated from the modified Taylor equation (2.126). It is important to note that the theoretical concentration distributions given by Equation (2.148) are relatively insensitive to changes in the magnitude of the dispersion coefficient. The dominant mass transfer mechanism is the advection due to the tidal velocity. Additional laboratory experiments on dispersion in an oscillating flow have been reported by Disko and Gedlund (1967) and Awaya (1969).

Numerical evaluations of Equation (2.148) have been carried out by Lee (1970) for a non-conservative substance (first-order decay) using freshwater flow, tidal parameters and a dispersion coefficient typical of the Delaware estuary near Philadelphia. The quasi-steady state concentration distributions, after 150 tidal periods, are shown in Figure 2.18 for both high and low water slack conditions. The tidal excursion λ equals 28,500 feet and the upstream limit of detectable concentration is seen to be of the order of 30,000 feet upstream of the injection station. The distribution curves of Figure 2.18 are relatively insensitive to changes in the magnitude of the dispersion coefficient, both upstream and downstream of the injection station. The concentrations upstream of the injection station are almost entirely due to tidal advection, while in the downstream direction the decay term K_d is the dominant quantity. The reference concentration C_o defined by Equation (2.147) has no physical significance in the case of non-conservative substances.

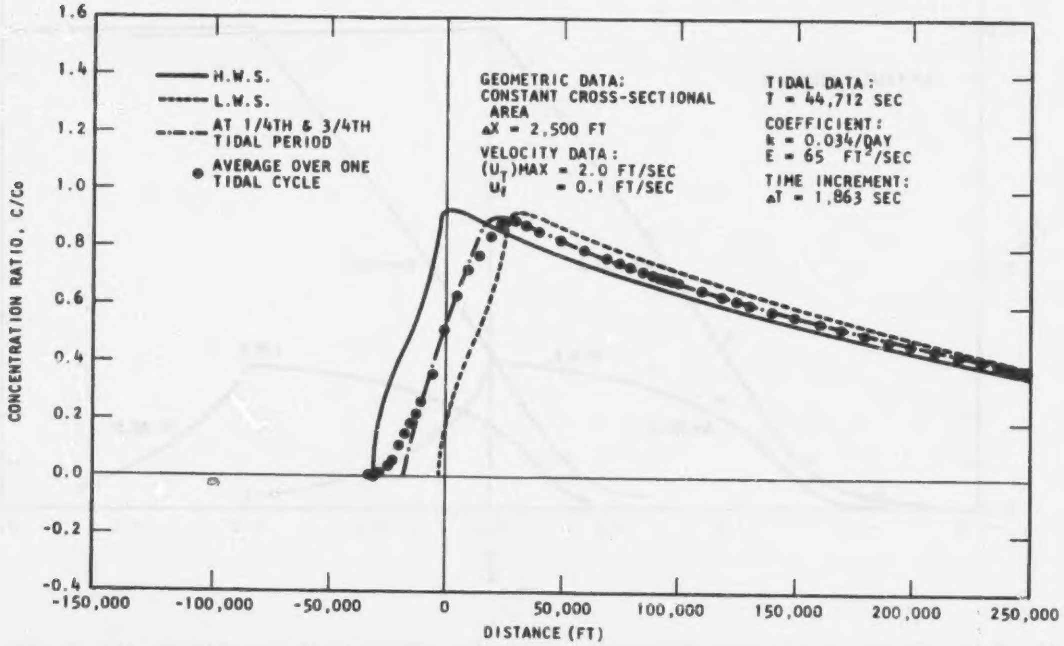


Fig. 2.18 Quasi-steady state solution of Equation (2.148) for non-conservative substance at high water and low water slack.

3.3 MASS TRANSFER EQUATIONS USING NON-TIDAL ADVECTIVE VELOCITIES

Because of the complexity of the unsteady, nonuniform flow in an estuary, it is not surprising that many investigators proposed mathematical models for the longitudinal distribution of pollutants which ignored the tidal advective velocity. Prior to 1950, the analysis of pollution in estuaries was based on the tidal prism exchange concept. This is illustrated by the work of Phelps and Velz (1933) in New York harbor and by the later work of Ketchum (1951a and 1951b). Ketchum divided the estuary into segments and assumed complete mixing within each segment during each tidal period. The state of knowledge as of 1950 was summarized in the proceedings of a colloquium on flushing of estuaries (Stommel, 1950).

3.3.1 Mass Transfer Equation: Time Average Over a Tidal Period

Arons and Stommel (1951) and Stommel (1953) were among the first to recognize the limitations of the tidal prism approach. They proposed the use of the one-dimensional mass transfer equation in which each term of Equation (2.133) is averaged over a period of time equal to the tidal period. Thus, the time-averaged mass transfer equation becomes

$$\frac{\partial \overline{C}}{\partial t} + U_f \frac{\partial \overline{C}}{\partial x} = \frac{1}{\overline{A}} \frac{\partial}{\partial x}\left(\overline{A}\overline{E}_L \frac{\partial \overline{C}}{\partial x}\right) + \frac{\overline{r}_i}{\rho} + \frac{\overline{r}_e}{\rho} \qquad (2.151)$$

where $\overline{C}$ is the concentration averaged over one tidal period, U_f is the non-tidal advective velocity due to freshwater inflow Q_f/A, and $\overline{E}_L$ is the time-averaged longitudinal dispersion coefficient. $\overline{A}$ is the time-averaged area and the source and sink terms are also time-averaged.

Stommel (1953) wrote the steady-state form of Equation (2.151) for a conservative substance by setting $\partial \overline{C}/\partial t = 0$ and assumed that the freshwater discharge $Q_f = \overline{A}U_f$ was a constant, thus

$$Q_f \frac{\partial \overline{C}}{\partial x} = \frac{\partial}{\partial x}\left(\overline{A}\overline{E}_L \frac{\partial \overline{C}}{\partial x}\right) \qquad (2.152)$$

The steady state refers to the fact that $\overline{C}$ does not change from one tidal period to the next if Q_f is a constant and if the boundary conditions for $\overline{C}$ are also constant. Inasmuch as all effects of mass transfer by tidal advection have been eliminated from Equations (2.151) and (2.152), such effects must appear in the time-averaged dispersion term. Stommel used Equation (2.152) in finite-difference form to determine $\overline{E}_L$ as a function of x from measurements of the salinity distribution in the Severn Estuary. He then calculated longitudinal concentration distribution curves for a pollutant introduced at an arbitrary section of the estuary. Pritchard (1952, 1954, 1958, 1960) developed similar mathematical models for conservative substances using time averages over a tidal period for both one- and two-dimensional conditions.

3.3.2 Mass Transfer Equation: Slack Tide Approximation

Mathematical models, based on a different non-tidal advective concept, have been formulated by O'Connor and DiToro (1964) and O'Connor (1965) for non-conservative substances. These studies have been concerned with the longitudinal distribution of BOD and dissolved oxygen resulting from instantaneous and continuous discharges of pollutants. It is important to note that O'Connor states that his mathematical models apply to concentration distributions at slack tide conditions rather than to concentrations which have been averaged over a tidal period. This is probably related to the fact that observations in many estuaries are available only at times corresponding to slack tide conditions. The terminology high water slack is used to indicate the change from flood to ebb and low water slack indicates the change from ebb to flood. In a strict sense, the time of slack tide is the time at which the advective velocity is zero. However, it was recognized that the elimination of the advective term in Equation (2.133) at slack tide would result in a loss of the entire flushing action. O'Connor, therefore, retained the non-tidal advective velocity due to freshwater inflow Q_f/A. This type of mathematical model will be called the slack tide approximation. Thus the appropriate form of Equation (2.133) is

$$\frac{\partial C_s}{\partial t} + \frac{Q_f}{A}\frac{\partial C_s}{\partial x} = \frac{1}{A}\frac{\partial}{\partial x}\left(AE_s \frac{\partial C_s}{\partial x}\right) + \frac{r_i}{\rho} + \frac{r_e}{\rho} \qquad (2.153)$$

The subscript s on the concentration variable and the longitudinal dispersion coefficient is a reminder that the concentration distribution is at slack tide. Equation (2.153) is the basic differential equation for O'Connor's mathematical models. The freshwater discharge Q_f and the longitudinal dispersion coefficient at slack tide E_s are assumed to be constant and independent of x. O'Connor obtained analytical solutions to Equation (2.153) for instantaneous and continuous injection of a pollutant for both constant and variable area estuaries, the latter for cases in which the area change is a linear, quadratic or exponential function of x.

The existence of two non-tidal mass transfer equations (i.e., the time average over a tidal cycle and the slack tide approximation) has resulted in a certain amount of confusion in the literature. This is due to a failure on the part of some investigators to discriminate between the two approaches. One reason for the confusion is that the mass transfer equations (2.151) and (2.153) are similar in that both contain an advective term due to freshwater inflow. The difficulty arises from the fact that the magnitudes of the longitudinal dispersion coefficients, E_L in the real time equation (2.133), $\bar{E}_L$ in the tidal-period-averaged equation (2.151) and E_s in the slack tide approximation equation (2.153), are not identical.

3.3.3 Analytical Solutions of the Non-Tidal Advective Mass Transfer Equations in a Uniform Estuary

Mass transfer equations based on the non-tidal advective concept are of two general types: the time average over a tidal period as given by Equation (2.151) and the slack tide approximation as given by Equation (2.153). There is no way for analytically predicting the dispersion coefficients in the non-tidal advective equations in a manner analogous to the modified Taylor Equation (2.126) or (2.127) in the real time system. This is one of the serious disadvantages of the non-tidal mathematical models. Whenever these models are employed it is necessary to determine the dispersion coefficients empirically for the particular reach under study by comparing solutions of the non-tidal mass transfer equation with observed concentration data. If the observed concentrations are for a non-conservative substance, such as a dye, BOD or DO, the solutions will contain one or more rate constants which depend on the nature of the source and sink terms for the substance whose concentration is being measured. These rate constants, together with the unknown dispersion coefficient, appear in the solution for the concentration distribution. Therefore there are several degrees of freedom, or combinations of parameters, which can be varied. It is not surprising that such multi-parameter models can be adjusted to match a given set of observations. It is difficult to claim that dispersion-coefficients or rate constants determined in this manner have any general validity.

Expensive and time consuming field tests, involving the injection and measurement of tracer substances, have been undertaken in the non-saline portions of estuaries for the purpose of determining dispersion coefficients. Similar tests have also been made in physical hydraulic models of estuaries. (See Chapter V, Section 3 for a discussion of certain similitude problems associated with dispersion in vertically distorted physical models.)

An understanding of the physical significance of the dispersion coefficients in the non-tidal mass transfer equations can be gained by comparing their solutions with the solution of the real time mass transfer equation under identical physical conditions. We consider the idealized estuary of constant cross-sectional area described in Section 3.2.6. The real time solution for a continuous injection of a non-conservative substance (first-order decay) is given by Equation (2.148), and the quasi-steady state concentration distributions are plotted as a function of x in Figure 2.16. In the following paragraphs the corresponding solutions for the non-tidal mass transfer equations are developed for a uniform estuary. The comparisons with the real time solutions are given in Section 3.4.

We consider initially the slack tide approximation. The appropriate form of Equation (2.153) for a constant-area estuary in which U_f , E_s , and K_d are constant is

$$\frac{\partial C_s}{\partial t} + U_f \frac{\partial C_s}{\partial x} = E_s \frac{\partial^2 C_s}{\partial x^2} - K_d C_s \tag{2.154}$$

The solution for a continuous injection at $x = 0$ at the rate w (pounds per second), beginning at $t = 0$, is given by Equation (2.146) with $U_T = 0$

$$C_s = \int_0^t \frac{w}{\gamma A\sqrt{4\pi E_s(t-\tau)}} \exp\left\{\frac{-[x - U_f(t-\tau)]^2}{4E_s(t-\tau)} - K_d(t-\tau)\right\} d\tau \tag{2.155}$$

This integral can be evaluated analytically in terms of error functions and exponentials

$$C_s = \frac{w}{2\gamma A\Omega} \exp\left(\frac{xU_f}{2E_s}\right) \left\{\left[\mathrm{erf}\left(\frac{x + \Omega t}{\sqrt{4E_s t}}\right) \pm 1\right] \exp\left(\frac{x\Omega}{2E_s}\right) - \left[\mathrm{erf}\left(\frac{x - \Omega t}{\sqrt{4E_s t}}\right) \pm 1\right] \exp\left(-\frac{x\Omega}{2E_s}\right)\right\} \tag{2.156}$$

where $\Omega = \sqrt{U_f^2 + 4K_d E_s}$. Where a choice of sign is indicated, the minus sign applies to values of $x > 0$ and the positive sign to values of $x < 0$

The steady-state spatial distribution of concentration is found by letting $t \to \infty$ and Equation (2.156) becomes

$$C_s = \frac{w}{\gamma A\Omega} \exp\left[\frac{x}{2E_s}\left(U_f \pm \Omega\right)\right] \tag{2.157}$$

Equation (2.157) reduces to very simple steady-state expressions for a conservative substance, $K_d = 0$ and $\Omega = U_f$,

$$C_s = \frac{W}{\gamma A U_f} \tag{2.158}$$

for $x > 0$ (downstream of injection section), and

$$C_s = \frac{W}{\gamma A U_f} \exp\left[\frac{xU_f}{E_s}\right] \tag{2.159}$$

for $x < 0$ (upstream of injection section). Equation (2.158) indicates a constant concentration downstream of the injection section and Equation (2.159) an exponentially decreasing concentration upstream of the injection section in a uniform estuary.

We consider next the mass transfer equation time-averaged over a tidal period. The appropriate form of Equation (2.151) for a constant-area estuary in which U_f , $\overline{E}_L$ and K_d are constant is

$$\frac{\partial \overline{C}}{\partial t} + U_f \frac{\partial \overline{C}}{\partial x} = \overline{E}_L \frac{\partial^2 \overline{C}}{\partial x^2} - K_d \overline{C} \tag{2.160}$$

From a mathematical viewpoint, Equation (2.160) and the slack tide approximation Equation (2.154) are identical. The difference is only in the meaning of the quantities $\overline{C}$ and $\overline{E}_L$ as opposed to C_s and E_s . The steady-state spatial distribution of concentration for the time-averaged mass transfer equation follows immediately from Equation (2.157)

$$\overline{C} = \frac{W}{\gamma A \Lambda} \exp\left[\frac{x}{2\overline{E}_L}\left(U_f \pm \Lambda\right)\right] \tag{2.161}$$

where $\Lambda = \sqrt{U_f^2 + 4K_d\overline{E}_L}$. A comparison of Equations (2.157) and (2.161) with the real time solution is given in Section 3.4.

3.3.4 Mathematical Models of Salinity Intrusion

A large number of investigators have used the non-tidal advective equations for the study of one-dimensional salinity intrusion in estuaries having varying degrees of sectional homogeneity. In dealing with salinity or chlorinity as the concentration variable, it is usually permissible to assume that the substance is conservative. This eliminates the source and sink terms and the associated rate constants in Equations (2.151) and (2.153). For an estuary in which certain salinity data is available and in which A and Q_f are known functions, the above equations can be used to determine dispersion coefficients. The choice of Equation (2.151) or (2.153) will depend on the nature of the salinity data.

A complete discussion of the many one-dimensional salinity investigations is beyond the scope of this report. Even a concise summary is difficult because of the different objectives of the various investigators. In general, the objectives may be classed as descriptive or predictive. Under the category of descriptive studies we include the use of salinity data and the conservative mass transfer equation to determine the longitudinal variation of the dispersion coefficient within the salinity intrusion region. A second mass transfer equation can be solved for the longitudinal distribution of a non-conservative pollutant introduced at a section within the salinity region. Under the predictive category we include investigations whose primary objective is the prediction of variations in the longitudinal salinity distribution due to changes in freshwater inflow, estuary geometry, or tidal range. A few examples are given in the following paragraphs.

3.3.4.1 Descriptive Studies The conservative form of the time-averaged mass transfer equation (2.151) can be integrated with respect to x (in the seaward direction) to obtain

$$\overline{E}_L = \frac{AU_f\overline{C} + \int_0^x A \frac{\partial \overline{C}}{\partial t}\, dx}{A \frac{\partial \overline{C}}{\partial x}} \qquad (2.162)$$

The evaluation of Equation (2.162) can be carried out in finite-difference form to determine $\overline{E}_L$ as a function of x for the period of time during which the salinity concentration data was obtained. Equation (2.152) is a special case of Equation (2.162) in which $\partial\overline{C}/\partial t = 0$. An expression for E_s similar to Equation (2.162) can be obtained by integrating the slack tide approximation Equation (2.153). Numerical evaluations of dispersion coefficients have been carried out by Kent (1960) in the Delaware, Burt and Marriage (1957) in the Yaguina (Oregon), Lawler (1966) in the Hudson, Cox and Macola (1967) in the Sacramento-San Joaquin Delta, Glenne and Selleck (1969) in San Francisco Bay, Dorrestein and Otto (1960) and Eggink (1966) in the Eems (Germany), and Boicourt (1969) in upper Chesapeake Bay. The dispersion coefficients obtained are characterized by large variations longitudinally with increasing values in the seaward direction. For example, in the northern arm of San Francisco Bay, Glenne and Selleck (1969) calculated values of $\overline{E}_L$ varying from 300 ft^2/sec (1 mi^2/day) to 18,000 ft^2/sec (56 mi^2/day).

3.3.4.2 Predictive Studies The principal difficulty in the development of predictive models for salinity intrusion is in the formulation of the boundary conditions for salinity. If x is measured in the landward direction from the mouth of an estuary, the upstream boundary condition for salinity as x becomes large, can be stated as

$$\begin{aligned} C &\to 0 \\ \frac{\partial C}{\partial x} &\to 0 \end{aligned} \qquad (2.163)$$

In the seaward direction it is obvious that the salinity must approach the constant value of salinity in the ocean; the difficulty arises because the longitudinal location at which the salinity becomes constant is a variable depending on freshwater inflow and tidal range.

Ippen and Harleman (1961) (see also Ippen 1966) analyzed a series of salinity distribution tests in a tidal flume at the Waterways Experiment Station. The experiments were conducted in a rectangular flume of constant cross section having a length of 327 feet. The upstream end of the flume has provision for the introduction of fresh water at a controlled rate. The downstream end is connected to a large tidal basin in which a constant salinity and a harmonic tide can be maintained. Observations of the salinity distributions were made for various combinations of tidal range and freshwater discharge.

Salinity distributions at high water slack and low water slack for three tests having the same basin tidal range are shown in Figure 2.19. The freshwater discharge for Test No. 2 is twice that of Test No. 16; and for Test No. 11 it is 2.8 times that of Test No. 16. The

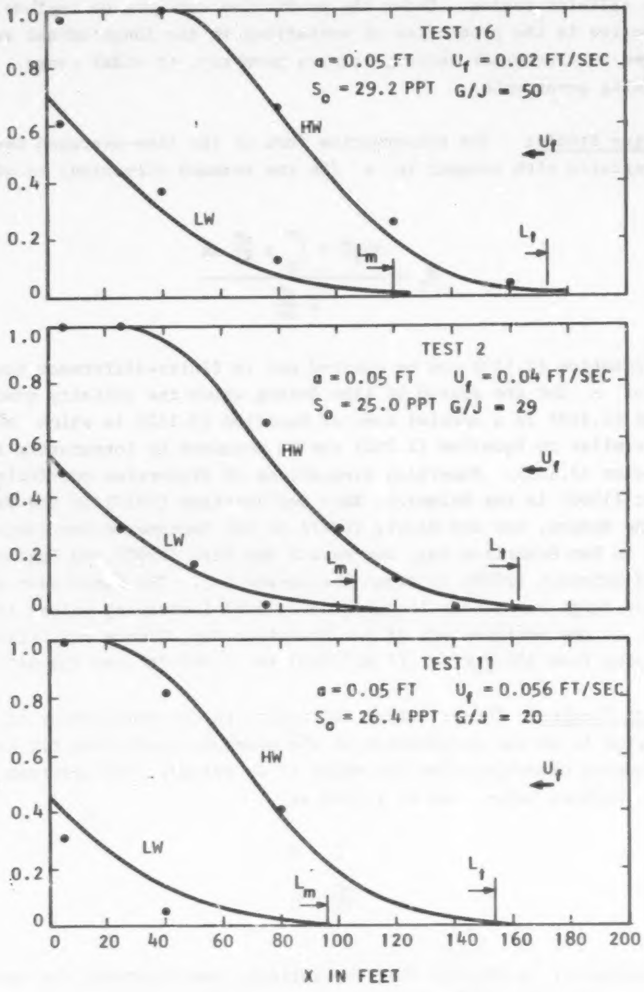


Fig. 2.19 Comparison of experimental and analytical salinity distributions for series I, tests 16, 2, and 11. Ippen and Harleman (1961).

change in the longitudinal position of the salinity distribution due to the increasing freshwater discharge is evident. Figure 2.19 also shows the validity of the upstream salinity boundary condition given by Equation (2.163) and the difficulty of specifying the seaward boundary condition. It was shown that the salinity distribution at low water slack could be advected upstream by a distance equal to the tidal excursion and that this distribution (shown by the solid lines in Figure 2.19) agreed with the salinity observations at high water slack.

Harleman and Abraham (1966) made use of this property and developed a mathematical model for the salinity distribution in a constant-area estuary based on the slack tide approximation. Under conditions of constant freshwater inflow and tidal range, Equation (2.153) reduces to

$$- U_f \frac{dC_{\ell s}}{dx} = \frac{d}{dx}\left(E_{\ell s} \frac{dC_{\ell s}}{dx}\right) \qquad (2.164)$$

where the subscript ℓs indicates the distribution at low water slack and x is measured in the landward direction from the mouth. Equation (2.164) may be integrated with respect to x, since U_f is a constant,

$$- U_f \, C_{\ell s} = E_{\ell s} \frac{dC_{\ell s}}{dx} + c_1 \qquad (2.165)$$

The integration constant c_1 is zero from the upstream boundary condition given by Equation (2.163). An equation for the salinity distribution is obtained by integrating Equation (2.165) a second time with respect to x. This requires that a function $E_{\ell s} = f(x)$ be specified, and that a boundary condition for the seaward end be formulated for evaluation of the second integration constant. The seaward boundary condition is obtained by assuming that the salinity distribution curve at low water slack can be extended in the seaward direction by a distance B to a point on the negative x axis where the salinity is equal to the ocean value C_o, thus

$$C_{\ell s} = C_o \text{ at } x = - B \qquad (2.166)$$

The dependence of $E_{\ell s}$ on x is assumed to be an inverse function of x of the form

$$E_{\ell s} = \frac{\left(E_{\ell s}\right)_o B}{x + B}$$

where $(E_{\ell s})_o$ is the dispersion coefficient for low water slack at $x = 0$. Under the above assumptions, Equation (2.165) can be integrated and the constant of integration evaluated from Equation (2.166),

$$\frac{C_{\ell s}}{C_o} = \exp\left[- \frac{U_f (x + B)^2}{2 \left(E_{\ell s}\right)_o B}\right] \qquad (2.167)$$

If the salinity is known at low water slack for at least two values of x, the parameters $(E_{\ell s})_o$ and B can be determined from Equation (2.167).

Figure 2.20 shows the parameters determined from Equation (2.167), and the agreement between the computed and observed salinities at high water slack after displacement of the low water slack distribution by a distance equal to the tidal excursion. The following empirical correlations were determined for the series of tests conducted at the Waterways Experiment Station:

$$\left(E_{\ell s}\right)_o = 0.008 \, U_o \frac{P_t}{A} \left(\frac{h}{a}\right)^{2.5} F_o^{\,2} \qquad (2.168)$$

$$B = 0.11 \frac{U_o T}{\left[\frac{P_t F_o^2}{Q_f T}\right]^{0.2}} \qquad (2.169)$$

where

U_o = maximum tidal velocity at $x = 0$
a = tidal amplitude at $x = 0$
h = mean depth
A = cross-sectional area
$F_o = U_o/\sqrt{gh}$
P_t = tidal prism (volume of sea water entering on flood tide)
Q_f = freshwater discharge
T = tidal period.

The salinity distribution predicted by Equation (2.167), using the parameters specified in Equations (2.168) and (2.169), has been verified by field measurements in the Rotterdam Waterway (Harleman and Abraham 1966). Salinity data for both 1908 and 1956 were used in the verification as shown in Figure 2.21.

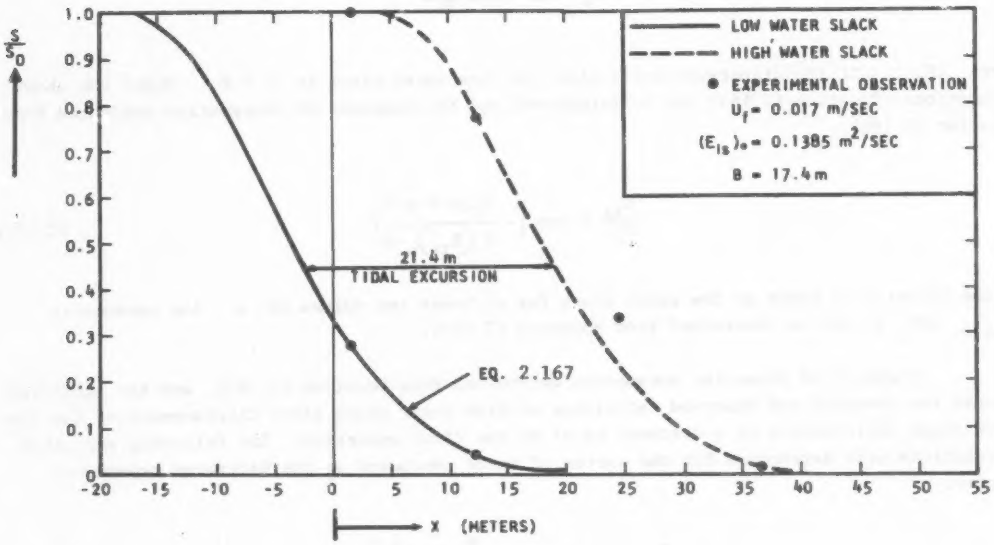
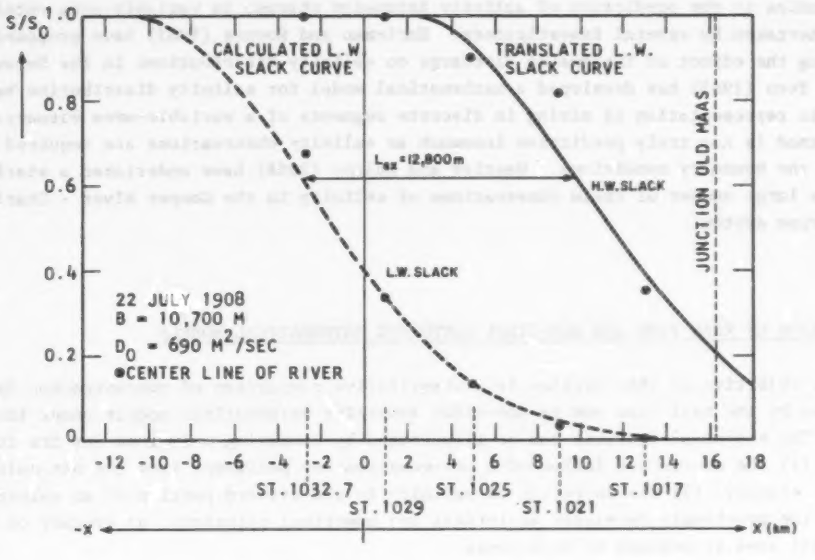


Fig. 2.20 Determination of salinity distribution parameters $(E_{ls})_o$ and B by comparison of Equation (2.167) and experimental data (Test No. 11).



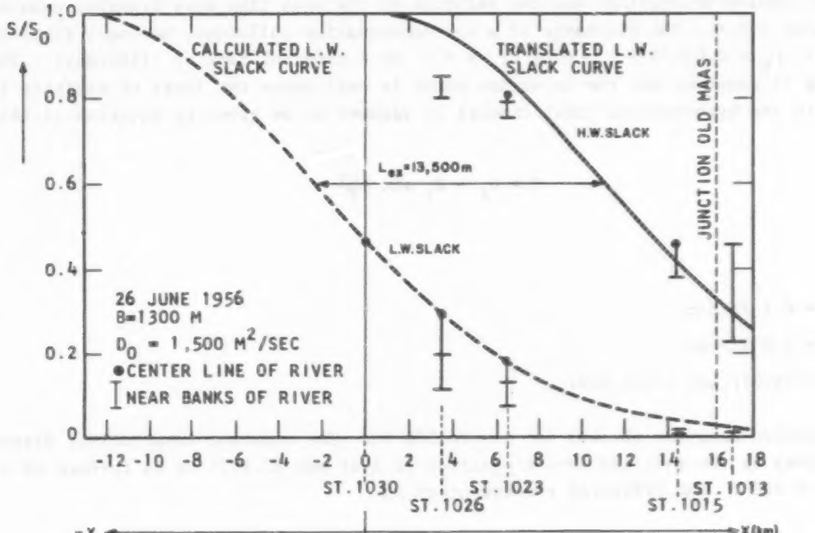


Fig. 2.21 Salinity data, Rotterdam Waterway.

Studies in the prediction of salinity intrusion changes in variable-area estuaries have been undertaken by several investigators. Harleman and Hoopes (1963) have proposed a method for predicting the effect of freshwater discharge on salinity distributions in the Delaware Estuary. Di Toro (1969) has developed a mathematical model for salinity distribution based on a Markov chain representation of mixing in discrete segments of a variable-area estuary. However, the method is not truly predictive inasmuch as salinity observations are required in order to establish the boundary conditions. Wastler and Walter (1968) have undertaken a statistical analysis of a large number of field observations of salinity in the Cooper River - Charleston Harbor estuarine system.

3.4 COMPARISON OF REAL TIME AND NON-TIDAL ADVECTIVE MATHEMATICAL MODELS

The objective of this section is a quantitative comparison of concentration distributions produced by the real time and by non-tidal advective mathematical models under identical conditions. The essential features can be illustrated by comparing solutions for the following conditions: (1) the continuous inflow of a non-conservative pollutant into the non-saline tidal portion of an estuary, (2) the intrusion of salinity in the seaward portion of an estuary. In order to use the previously developed analytical and numerical solutions, an estuary of constant cross-sectional area is assumed in both cases.

3.4.1 Continuous Inflow of a Non-Conservative Pollutant

The problem description and the solution of the real time mass transfer equation are given in Section 3.2.6. The discharge of a non-conservative pollutant, having a first-order decay constant $K_d = 0.034/\text{day}$, occurs at $x = 0$ at a constant rate w (lbs/day). The cross-sectional area is constant and the injection point is well above the limit of salinity intrusion. The velocity in the hypothetical tidal channel is assumed to be given by Equation (2.145),

$$U = U_f + U_T \sin \frac{2\pi t}{T}$$

where

$U_f = 0.1$ ft/sec

$U_T = 2.0$ ft/sec

$T = 44{,}712$ sec (12.4 hrs).

The tidal excursion Equation (2.149) is $\lambda = 28{,}500$ ft. The constant longitudinal dispersion coefficient given by the modified Taylor equation (2.126) and (2.127) is 65 ft²/sec (0.2 sq mi/day) for $n = 0.028$. The reference concentration is

$$C_o = \frac{w}{\gamma A U_f}$$

The real time solution is given by Equation (2.148) and the quasi-steady state concentration distributions at high and low water slack are plotted in Figure 2.18. The corresponding steady-state solution for the slack tide approximation is given by Equation (2.157). This equation can be written in terms of the reference concentration C_o as follows:

$$\frac{C_s}{C_o} = \frac{U_f}{\Omega} \exp\left[\frac{x}{2E_s}\left(U_f \pm \Omega\right)\right] \qquad (2.170)$$

where the negative sign applies to $x > 0$ and the positive sign to $x < 0$ and $\Omega = \sqrt{U_f^2 + 4K_dE_s}$

The comparison of the real time solution and the slack tide approximation is shown in Figure 2.22, using the same numerical values in both solutions. According to the slack tide approximation, there is essentially no concentration distribution upstream of the injection section ($x = 0$). At $x = -3000$ ft., or ten percent of the tidal excursion, the concentration predicted by Equation (2.170) is $C_s/C_o = .01$ which is too small to show in Figure 2.22. The real time solution predicts measurable concentrations over a distance of 30,000 feet or approximately 6 miles upstream of the injection section. In the downstream direction, the slack tide approximation falls essentially between the high and low water slack distribution of the real time solution.

Inasmuch as the dispersion coefficient E_s in the slack tide approximation is not predictable in advance, we may inquire whether it is possible to find a constant value of E_s which will result in a reasonable agreement with the real time solution, both upstream and downstream of the injection section. The result of two trial values of E_s of 1200 ft²/sec (3.75 sq mi/day) and 2250 ft²/sec (7 sq mi/day) is shown in Figure 2.23, the latter value being 35 times larger than the dispersion coefficient used in the real time solution. It can be seen that the shape of the concentration distributions are quite different and no single value of E_s will bring the two mathematical models into agreement. The same difficulty arises with respect to the time-averaged mass transfer equation since Equation (2.161) is of the same form as Equation (2.170).

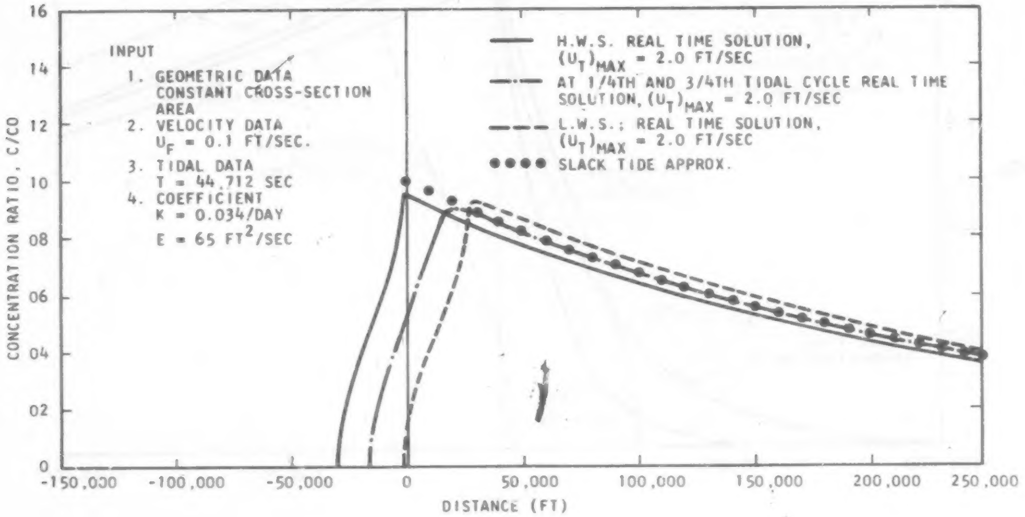


Fig. 2.22 Comparison of real time solution, Equation (2.148) with slack tide approximation, Equation (2.170) for continuous inflow of a non-conservative pollutant.

3.4.2 Salinity Intrusion

The example used for this comparison is described in Section 3.2.4.2 and is based on salinity intrusion data for the Rotterdam Waterway. The agreement between the observed salinity distributions and calculated values using the real time equations is shown in Figure 2.16 where

$$E_L{}' = 13{,}000\ (1 - x/L)^3\ ,\ [\mathrm{ft}^2/\mathrm{sec}] \qquad (2.131)$$

It is desired to compare the longitudinal dispersion coefficients obtained from the non-tidal mathematical models, using the same salinity data, with the above values of $E_L{}'$ in the real time model.

The dispersion coefficient in the time-averaged mass transfer equation can be determined as a function of x from Equation (2.162) by using the time-averaged salinity distribution data of Figure 2.16. In the Rotterdam Waterway, the cross-sectional area is essentially constant and the salinity data was obtained during a period of time when $\partial\bar{C}/\partial t = 0$. Therefore, Equation (2.162) reduces to

$$\bar{E}_L = \frac{U_f\bar{C}}{d\bar{C}/dx} \qquad (2.171)$$

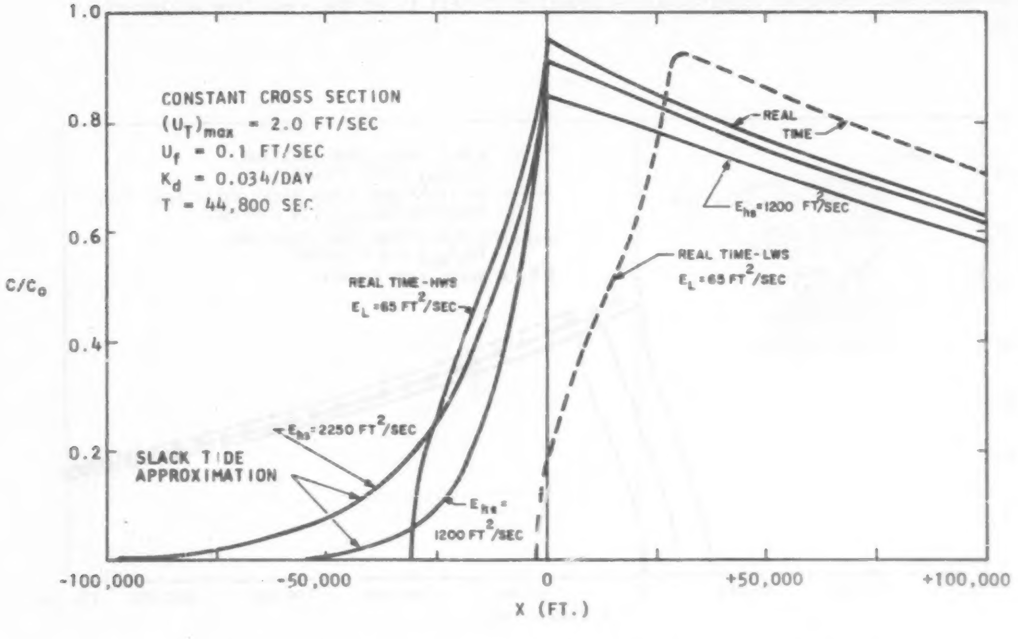


Fig. 2.23 Comparison of real time solution, Equation (2.148) [E_L = 65 ft²/sec], with slack tide approximation, Equation (2.170) [E_{hs} = 1200 and 2250 ft²/sec], for continuous inflow of a non-conservative pollutant.

The corresponding form for the slack tide approximation is

$$E_s = \frac{U_f C_s}{\partial C_s/\partial x} \qquad (2.172)$$

It is apparent that two sets of $E_s = f(x)$ can be obtained from Equation (2.172) depending on whether the salinity data for high or low water slack is used.

The results of applying Equations (2.171) and (2.172) to the Rotterdam Waterway data are shown in Figure 2.24 where $\bar{E}_L$ and E_s (high and low water slack) are plotted as functions of x. In addition, the real time dispersion coefficient E_L' given by Equation (2.131) is plotted as a function of x for comparison. It is apparent that significant differences exist between the real time and the non-tidal dispersion coefficients in salinity intrusion regions.

3.5 SUMMARY AND CONCLUSIONS

The basic mathematical framework for estuarine water quality is a mass transfer equation, alternatively known as a conservation of mass equation, a mass balance, a convective-diffusion or a convective-dispersion equation. This section of Chapter II has dealt with the one-dimensional form of the mass transfer equation with particular emphasis on the hydrodynamic aspects of the mathematical model. The general form of the one-dimensional equation is given by Equation (2.95). The hydrodynamic aspects, as here defined, are contained in the first three terms of this equation which relate to the temporal and spatial variation of area, velocity and longitudinal dispersion coefficient. The water quality aspects are contained in the remaining source and sink terms in the mass transfer equation. The dependent variable is the concentration of a substance in the water mass whose distribution in space and time is to be determined. The concentration of substance may refer to chemical and/or biological components. In general, a coupled set consisting of N mass transfer equations is required in order to define the water quality state of an estuary in terms of N water quality parameters.

The section is divided into three parts; Section 3.2 treats the mathematical models in real time (i.e., following the tidal motion), Section 3.3 deals with the mass transfer equations using non-tidal advective velocities, and Section 3.4 presents a comparison of these two basic types of water quality models. A brief summary of the mathematical models is given below.

3.5.1 Mathematical Models in Real Time

The real time mass transfer equation requires some knowledge of the tidal motion in the estuary. The input to the mass transfer equation is the specification of the cross-sectional area and velocity as functions of x and t. Considerable latitude is possible in the completeness and accuracy in which the tidal information is supplied. In general, the analytical efforts are in inverse proportion to the amount of field data available. Three approaches are described in Section 3.2.3.

(i) Calculation of the tidal characteristics by simultaneous solution of the continuity and momentum equations. This approach requires a minimum amount of field data; techniques involving simultaneous solution by finite-difference equations are well developed.

(ii) Calculation of the tidal characteristics by cubature. This approach requires extensive field data on the distribution of tidal amplitude and phase. The continuity equation is solved

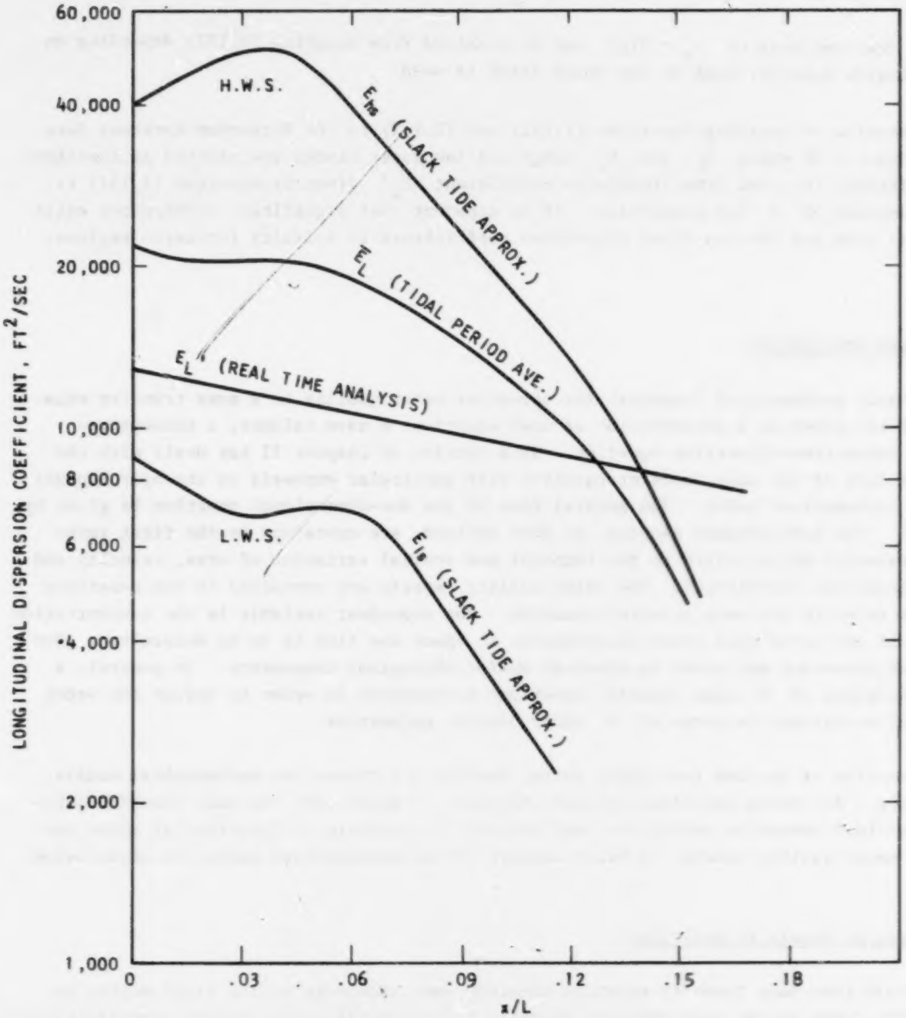


Fig. 2.24 Comparison of longitudinal dispersion coefficients obtained from analysis of Rotterdam Waterway salinity data (Stigter and Siemons 1967).

by finite-difference techniques to obtain the tidal velocity.

(iii) Assumption of a sinusoidal or harmonic representation of the tidal velocity in the form of Equation (2.122). Field data on the maximum values of tidal velocity are required and no analytical techniques are employed.

The first two approaches may contain important nonlinear information on the tidal motion which is characteristic of many estuaries. Such nonlinearities take the form of unequal magnitude and duration of ebb and flood velocities. In general, the trade-off between the time and expense of tidal analysis versus field measurement of tidal quantities is heavily in favor of analysis.

Longitudinal dispersion in the real time mass transfer equation is discussed in Section 3.2.4. It is important to distinguish between longitudinal dispersion in estuarine regions of uniform water density as opposed to regions in which density gradients exist due to salinity intrusion. A modified form of the Taylor dispersion equation (2.126) and (2.127) is used to determine the magnitude of the longitudinal dispersion coefficient E_L in regions of uniform density. The magnitude of E_L depends on the local value of the maximum tidal velocity, hence any of the techniques for determining the tidal hydraulics provides the necessary information to find the dispersion coefficient in the uniform density region. The determination of the longitudinal dispersion coefficients in the salinity intrusion region requires field data on salinity distribution. The magnitudes of E_L' are found by fitting the solution of the conservative substance mass transfer equation to the observed salinity data. The tidal hydraulic solution previously obtained provides the advective velocity input to the mass transfer equation for salinity.

3.5.2 Mass Transfer Equations Using Non-Tidal Advective Velocities

Two forms of the mass transfer equation using non-tidal advective velocities are discussed in Section 3.3. In one case the real time mass transfer equation is simplified by time averaging over a tidal period. All concentrations refer to averages over the tidal period, and the advective velocity reduces to a small value associated with the non-tidal discharges such as freshwater inflow. In the other case, a simplified mass transfer equation is obtained from the real time equation by considering concentration distributions only at times of slack tide. The advective velocity is arbitrarily set equal to that associated with non-tidal discharges. The two models are mathematically similar although the concentration distributions derived from them are quite different. Each of these simplifications of the real time mathematical model has the effect of incorporating the mass transfer effects associated with the advective tidal motion into the dispersive term. The dispersion coefficients in the non-tidal mass transfer equations must be determined empirically, both in the constant density and salinity intrusion regions.

3.5.3 Conclusions

A state-of-the-art review should have as a primary objective the establishment of guidelines for future developments in the field. Within the inherent limitations of one-dimensional mathematical models for estuarine water quality, two choices appear to be open: (i) to continue development of the non-tidal advective models; (ii) to continue development of the real time models. Water quality models based on the non-tidal advective concepts were developed in the pre-computer era They were logical extensions of the Streeter-Phelps approach for streams and rivers. The difference is in the inclusion of a dispersion term which is the only mechanism by which mass can be transported upstream in a non-tidal model. The non-tidal mass transfer differential equation can be solved in a straightforward manner, at least for estuaries in which the geometry is a simple function of x . No analysis of the estuary tidal motion is required and the time scale, of the order of a tidal period, seemed adequate for many water quality investigations. There are, however, numerous examples of estuarine problems in which the analytical solutions requiring constant coefficients and simple geometric relations are inadequate. In these cases, finite-difference computer solution techniques have been developed. It is important to question whether the continued development of the non-tidal advective models is a reasonable exploitation of the capabilities of the computer era.

The longitudinal dispersion coefficient in the non-tidal mathematical models is an elusive quantity requiring an ad hoc empirical determination for each situation under investigation. Its determination has been the subject of many expensive and time consuming studies involving dye injection or other tracer observations both in the field and in physical hydraulic models. Thus the analytical simplifications gained by ignoring the tidal motion are more than offset by the difficulties of determining an appropriate dispersion coefficient. This is especially important in tidal regions where salinity cannot be used as a conservative natural substance. In this context Figure 2.23 shows the essential point of the argument as applied to the constant density tidal region. The dispersion coefficient for the real time mathematical model is predicted by the modified Taylor equation; however, the transport of mass upstream of the injection point is almost entirely by the mechanism of tidal advection. The concentration distribution produced by the real time model is relatively insensitive to variations in the predicted dispersion coefficient. In the non-tidal mathematical model an inflated dispersion coefficient of the order of 35 times the real time value is required to produce an upstream transport, which is at best a poor approximation to the real time distribution. It is concluded that the importance of longitudinal dispersion decreases as the accuracy of description of the advective motion increases.

Further ambiguities in the non-tidal-advection dispersion coefficients have been illustrated in the salinity intrusion region. Figure 2.24 shows the wide variation in the magnitudes of non-advective dispersion coefficients obtained by analyzing salinity data (i) at high water slack, (ii) at low water slack, and (iii) as a time average over the tidal cycle. It is apparent that dispersion effects, and especially dispersion coefficients, cannot be discussed in an abstract manner. They are essentially defined by the formulation of the mathematical model in that the effective dispersion always depends on the way in which the advective motion is described.

Technical developments in the field of tidal hydraulics have provided the capability of treating the tidal advection in the mass transfer equation in a satisfactory and unambiguous manner. The use of real time water quality models eliminates uncertainty associated with arbitrary dispersion coefficients in the non-tidal models. This should permit future developments to center on the important and difficult problems relating to generation and decay of non-conservative substances and the interaction of chemical and biological substances in simultaneous mass transfer equations.

The above considerations suggest that the time scale associated with the mathematical water quality model is not necessarily determined by the time scale of interest in a water quality problem. The small time scale of the real time models should be considered as a necessary solution technique which avoids the ambiguous coefficients associated with the non-tidal advective models. The choice is again one of a trade-off between the time and expense devoted to analysis as opposed to the time and expense of the additional field work, such as special dye dispersion tests, required by the large time scale, non-tidal water quality models. In addition, increasing concern with the total ecological system makes it difficult to ignore the real "time of travel" associated with the tidal motion.

The real time water quality model makes it possible to consider estuary pollution control by time-dependent effluent discharges. For example, a source of pollution located within one tidal excursion of the estuary mouth could make use of a six hour detention basin in order to discharge at twice the average rate during the period of ebb tide.

Although these conclusions have a strong bias in favor of the real time mathematical model it is not proposed that all existing or future water quality models be reformulated on this basis. There will continue to be a place for the simpler non-tidal advective models in the analysis and prediction of estuarine water quality. For example, in a major estuary study, both the real time and the non-tidal advective models could be formulated initially. Solutions for both models could be obtained for a single effluent source undergoing a simple first-order decay. The real time model could then be used to verify the hydrodynamic aspects of the non-tidal model through the choice of non-tidal dispersion coefficients to a desired degree of agreement with the real time solution. Thus the formulation and solution of the real time problem is an "analytical dye dispersion test" which replaces the prototype or hydraulic model "dye dispersion test" previously used to verify the non-tidal mathematical model. In the remainder of the study, simultaneous non-tidal advective models could be used to consider the interaction of water quality substances and multiple sources of pollution.

Solutions from the real time model may also be used to check finite-difference formulations of water quality models. The finite-difference technique can be checked by applying it to an estuary of uniform geometry for which analytical solutions in real time are available.

The details of finite-difference solution techniques are not within the scope of this chapter. However, reference is made to several studies involving the formulation of the real time mass transfer equation in finite-difference schemes. Bella and Dobbins (1968) presented the results of finite-difference calculations for BOD and DO profiles in the constant density portion of a hypothetical constant-area estuary having a sinusoidal tide. Their results are compared with solutions obtained from the steady-state, non-tidal advective mass transfer equations. Dornhelm and Woolhiser (1968) developed a finite-difference scheme for a hypothetical estuary (whose area varies as a linear function of x) with a sinusoidal tide. Certain difficulties with boundary conditions were encountered. In both of the above investigations the numerical values of the real time dispersion coefficients were arbitrarily assigned. In other words, the link between the magnitude of the dispersion coefficient and the tidal motion was not considered. Orlob et al. (1967) and Orlob (1968) have studied water quality problems in San Francisco Bay and the Sacramento-San Joaquin Delta area. The problem includes two-dimensional components due to lateral variations in embayments such as San Pablo and Suisun Bays. The computational scheme consists of a link-node network configuration of uniform flow channels. The real time finite-difference model considers tidal advection and dispersion in the uniform channel links between nodes. All non-advective and dispersion aspects of the mass balance such as decay and surface transfer are assumed to be concentrated at the nodal junctions. The dispersion coefficients and the rate constants of the various source and sink terms must be adjusted to match field data. Callaway et al. (1969) have proposed the application of this type of model to the lower portion of the Columbia River.

An extensive study of the real time mass transfer mathematical model has been undertaken by Lee (1970). Finite-difference formulations of the continuity, momentum and mass transfer equations have been developed for variable-area estuaries of arbitrary geometry. This permits inclusion of nonlinear tidal advection, multiple pollution sources, and time-dependent freshwater inflow. The real time longitudinal dispersion coefficients are related to the tidal motion, through salinity observations in the salinity intrusion region and through the modified Taylor dispersion equation in the constant density tidal region. Water quality parameter observations in the Potomac, Delaware and James estuaries are used for comparison with the analytical results. Preliminary results have been published by Harleman et al.(1968) for the upper freshwater tidal reach of the Potomac and compared with the field observations of Hetling and O'Connell (1966). This is essentially a demonstration of the validity of an "analytical dye dispersion test".

In conclusion, it is suggested that the state-of-the-art is such that ambiguities regarding the hydrodynamic (i.e., advective-dispersion) aspects of mass transfer in estuaries should no longer be accepted in one-dimensional water quality models. Undoubtedly, future developments will continue both in the real time and in the non-tidal advective models. The rapidly increasing capability of high-speed computers suggests less reason for future reliance on the non-tidal models. When they are used, it is hoped that their limitations and their relation to the real time models will be understood.

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DISCUSSION

PRITCHARD: In this first section we deal with the basic equations in a development that might serve as a three-dimensional model. Now I went to some extent philosophically here to discuss some questions concerning averaging that I feel, if not properly treated, can get us off on the wrong foot with the basic equations. Also, I spent some time in trying to start with first principles and show what is neglected. I know that many of the engineers are concerned with conservation of these properties over a cross section or seaward element extending from surface to bottom, and apply the basic principles to that finite element. I find that I sometimes miss terms when I do that. So my approach to the bookkeeping starts with the basic principle which was really developed to be applied to a moving particle of water properly defined, and then integrating these equations over space, and I think it may be that one is less likely to miss some important terms.

We note a couple of things about these equations. One is that we have these stress terms which we need to find out how to treat. And then what I have done with respect to the pressure term is to try to put it into a form that people who have used one-dimensional and two-dimensional models would feel more at home with, that is, to put the pressure term in terms of the slope of the sea surface. When we do this, we've got to recognize that in what I consider real estuaries, estuaries that have freshwater inputs sufficient to give a field gradient in salinity, there is a distribution of density, both vertical and horizontal, and that this distribution of density leads to an internal slope in the pressure field. An internal slope in the pressure field introduces into the pressure force term an additional slope, the slope of the pressure surfaces relative to the sea surface, which I have labeled here as $i_{1,p,\eta}$ meaning the slope of a pressure surface in the x_1 direction referred to the surface, the surface being η.

These equations are then coupled with the equation of continuity and with the vertical equation which can be used to compute the internal slope of the pressure field. This kind of computation is a classical one in oceanography. It's done every time oceanographers compute geostrophic currents to determine essentially the slope of the isobaric surfaces. It is not stated that way, but the technique for carrying out the integral given on the right side of (2.21) and (2.22) is readily available in oceanographic texts. So those equations must be used as auxiliary equations.

Now, these equations as they stand have more unknowns than there are equations. For one thing, you've got to know the time-dependent density field to compute the internal slope of the pressure surfaces, so that it's necessary in any case, not only to solve simultaneously the conservation of mass and the conservation of momentum, but you must also simultaneously solve the time-dependent distribution of salinity. You've got to feed that back in, as density is dependent on salinity, to compute the density field and to compute the internal pressure field.

What I've done then is to attempt to argue for some further simplification of these equations. That leaves us with the Equations (2.27) and (2.28). We really have no direct evidence that these equations can be further simplified. They represent equations with three velocity components, as a function of time and three spatial coordinates, and the surface elevation, as a function of position and time. being the things that we want to get out of them.

Then I have given a development of what you might call the salt balance equation in three dimensions. Now it has been argued from studies that have been done in two dimensions that the more one knows about the details of motion, the less concerned one has to be with the diffusion terms. I think that this is probably true in the horizontal components. These terms arise out of the cross products of the horizontal velocity deviations, the gradients of these terms, and they arice out of averaging the advective terms, so that if you know more about the advective terms it's obvious that the diffusion terms become less important. I think that if you are going to deal with three dimensions, you can't treat the vertical term in the same way. It becomes important when we have to talk about the vertical third dimension. But I have argued that in both the momentum equation and the salt balance equation the horizontal eddy viscous terms and the horizontal eddy diffusion terms can probably be neglected as long as we are talking about ensembles and the ensemble-averaged equations.

Finally, one then arrives at Equations (2.35) and (2.36) which are the two horizontal components of the equation of motion in three dimensions reduced about as far as I think we have any basis for reducing them at the present time, and the salt balance equation (2.37) also reduced about as far as I think we have any basis for reducing it. I want to point out that these equations still contain a vertical turbulent viscous term, a vertical diffusion, and also that the equations of motion contain this term which involves the internal variation in the pressure field because of the distribution of density. I want to point out also that the size of that term is not revealed by looking at the vertical distribution, as Rattray has shown. This term is a term that leads to, in what I would call strong estuaries, there being a shear positive towards the ocean. The net effect is that there is essentially a shear in the time-dependent vertical velocity field leading to a tidal-averaged motion which is essentially two-layered, with motion towards the ocean and towards the land. I want to emphasize that you can't be fooled into using the vertically averaged equations in which that part of the pressure term is omitted simply by saying that this is a well-mixed estuary, because salinity hardly varies from top to bottom. You may have an estuary which is sufficiently well-mixed vertically, as far as salinity goes, but which will not be well-mixed as there is a shear in the velocity field. There still will be this two-layered flow. A good case of this is the study of the Mersey by Bowden which was considered as a classical case of a well-mixed estuary, but he showed it very definitely had a vertical shear in the velocity field, and had a flow pattern as I have described.

Then in order to complete the ensemble of equations, you've got to impose certain boundary conditions, among these certain integral conditions, that is, conditions on the equations integrated vertically and across the cross section. These integral forms of the equations provide additional terms, for instance Equation (2.40) provides an additional relationship which allows the computation of η coupled with the other equations, and so on.

We still end up in this situation having some unknown terms, for instance the vertical eddy viscosity which I've labeled ν_3 and the vertical eddy diffusivity which I've labeled K_3. I have talked about some evidence for the vertical variation in the eddy diffusivity based on some data that I got in the James, and compared it with some data that was taken by Bowden in the Mersey.

I'd like to point out that this is one of the really big unknowns, and this is an area in which we really need to have some work done. And that is: how do we relate the vertical eddy viscosity and the vertical diffusivity to known or computable parameters? And to me it is a very important unknown.

Equation (2.58) is a vertically-averaged equation of continuity expressing the conservation of mass, which can also be shown to reduce to the fact that the horizontal divergence of flow must equal the time rate of change, the rise and fall, of the sea surface, that is, Equation (2.59). It represents continuity in two dimensions. Then I've treated the conservation of momentum in the same way, but in this case you can't a priori drop the cross-product terms. We treat the two-dimensional equations of motion, in which we get some terms which involve the vertical mean average of cross products of the deviations, like $u_h' v_h'$ and $(u_h')^2$, which depend on the vertical shear of the motion. In estuaries in which the mean internal pressure slope is important, there's going to be a vertical shear and these cross-product terms are likely to be important. One has boundary values for the vertical stresses. One of these is the wind stress, $\tau_{w,x}$ and $\tau_{w,y}$, and the other is the bottom stress which I have accepted as being reasonably expressed in terms of a Chezy-type equation. I've argued about the size of these viscous terms (or these terms that have the appearance of a Reynolds stress term but which really involve the fact that you are vertically averaging a vertically varying velocity field) and said that, well, maybe you can express these in the same way you expressed the Reynolds stress terms before, writing the vertical-mean value of these velocity deviations in terms of a component of the deformation tensor and some sort of an eddy coefficient. But these eddy coefficients now are quite different from those in the three-dimensional equation. They are not simply the average of a cross-product of turbulent deviations, but are averages which involve the fact that the real mean motion, the deterministic part of the motion, varies through the depth. I don't know how to treat these. I don't know whether we know enough about them. Don [Harleman] has some ideas from some of his flume studies, but for the moment I'm just saying that I hope they're small enough to be neglected.

Let's consider the case where they're small, Equation (2.66) and (2.67), which says that the acceleration, both local and field, of the vertical-averaged velocity field is equal to the sum of a pressure term which involves gravity times the gradient of the slope of the surface plus the vertical-mean value of the slope of the isobaric surfaces relative to the sea surface, a term involving an atmospheric pressure gradient, the coriolis term, wind stress term and the bottom stress term.

One can't really argue that these terms, the average of the internal slope of the pressure surface, are small, even in this averaged case, even in this two-dimensional case. In the James, for instance, this kind of process represents about 36% of the mean of the absolute magnitudes of the surface slope over a tidal period. This is a term that doesn't vary much with the tide, that is, the tide causes both of these things to vary, the surface of the water and the pressure surface. Over the tidal cycle this internal slope doesn't vary, so that it's there at all phases of the tide. So I don't think you can neglect it, even in the vertically averaged equations for most real estuaries. Now, there are bays, lagoons, and other kinds of waterways in which the input fresh water is sufficiently low so that salinity doesn't have much horizontal variation, and they're shallow, so that the type of vertical average that has been proposed by Jan Leendertse here probably is valid. But I don't think it applies to the estuaries along the east coast of the United States.

RATTRAY: I'd like to reinforce the statement about the importance of the internal density field in governing the motion, and particularly the rate of dispersion of any quantity introduced. I think this, as far as I have been able to see in many of the studies that have been going on in the recent past, has been overlooked, and the effect seems to be important in almost all cases where they do have salinity distributions, estuaries for example. Again, it is not true that you can look at the vertical salinity profile and on the basis of that alone say anything about the vertical profile, on the average. Looking at the salinity distribution won't uniquely give you the mean velocity distribution nor the other way around, so that one has to look at it in a little more detail. Particularly the depth is important: the same density difference will drive a stronger circulation as the estuary becomes deeper. So in these very shallow situations the density fluctuations due to the salinity may not be very important, but as you get into deeper bodies of water it will be. The Mersey, for example, was a case in point. Certainly Puget Sound is a case in point.

In the equations that have been derived here, I'm very happy to see the detail that has been gone into, because I think this is an important starting point which will show quite clearly the shortcomings of various models that have been proposed, and where they might be improved.

I have maybe a question, Don. I haven't really been able to digest it this fast, but with what you've done with two-dimensional estuaries, it doesn't seem that you have a closed set of equations--now that you've put in some of the terms that should have been included--equations that you can't really solve without going three-dimensional.

PRITCHARD: Well, I think it is closed from the standpoint that there are some integral boundary conditions that you've got to take just as you do in the three-dimensional case, to give you some additional terms which allow you to close the solution for η, you see. Because η is not dependent on three dimensions; it's only dependent on two effective dimensions.

RATTRAY: Well, I guess I see what I am really after. You use Reynolds stresses for the vertically integrated difference terms. I wonder if you think there is any such real eddy coefficients that one can reasonably define and then use from one situation to another, as the river conditions and whatever might change.

PRITCHARD: You notice that in the next paragraph I say I don't know how to treat these and I am going to treat the case where you can forget about them. But now I think Don [Harleman] might have some comments on this from his work at Vicksburg, where he puts fresh water in one end of a flume and salt water in the other, then vibrates a frame of what you might call roughness elements in the flume, and gets something of a convective transport picture.

RATTRAY: That's part of it. The other is that you have internal pressure fields. How do you get those in a vertically integrated model?

PRITCHARD: That's the $i_{x,p,\eta}$ and $i_{y,p,\eta}$ averaged over h. The way you get this is to have a simultaneous solution of the vertically averaged salinity balance equation. Again what do you do about diffusion in that case? Even if you might neglect the horizontal terms involving these vertical averages of the velocity deviations that arise out of vertical shear--because, even if those terms individually might be strong, their gradients may not be large, as they appear in the dynamic equations or the equations of motion--I don't think the same kind of arguments can be made necessarily about the cross-products involving velocity and salinity. You can't *a priori* say just because this kind of process is small in one equation then it is in all of the others. So that you do have the question of what can you do about these diffusion terms. At least, I think that it is not a question of how fine you take the velocity field because you are not taking the vertical variation in the horizontal velocity fine at all in this vertically averaged equation.

So I think we have problems here, but let's assume that through experiments and such evidence, we get some way of relating the diffusion processes to known or computable terms, and we can solve these equations simultaneously in the two dimensions. This means that you have to take in each time step the salinity you get, and compute a slope term. You'll get a value for this vertical mean of the internal slope, simply by taking the vertical-mean density field using the salinities you computed each of these time steps, and using the conventional arguments about how thick that column of water must be to have the same pressure at the bottom.

RATTRAY: How do you get the horizontal advection of salt correct, which is usually a significant fraction of the horizontal salt flux, in the vertically averaged set of equations? Don't you have to know what the vertical profile velocity is?

PRITCHARD: I agree with your problems. They are problems that have worried me. But what I am saying is if we are going to try to go on, quite frankly as I've developed it now, I think we are going to the three-dimensional equations.

RATTRAY: That's what I wanted to get you to say.

PRITCHARD: After all, we're writing this as a state-of-the-art report, and we've got to have in here relationships which can be compared to models that the federal people have to look at in terms of having been presented as ways to solve their problems. And I wanted to get the equations in the forms that are nearest to the ones that they have been faced with, in evaluating and perhaps using, and then say: well look, these equations miss these terms. That's the main purpose of the exercise here. I think that it will be well worthwhile to try some two-dimensional models with this mean of the internal pressure field in them just to see what difference it makes in those kinds of equations. But ultimately I think we have got to go to the three-dimensional equations, which means a lot more computer time.

LEENDERTSE: I would like to make a comment on this slope term. Assuming now that it doesn't change very much, let's say if you have a certain amount of fresh water to salt water, a tidal excursion at the inlet of, say, five miles or so, you only get very small time variations so that effectively this gives a fixed value of this slope in your computations. Now you never know in actual computations what the different levels really are between the gauges which you have, so you may not be able very often to distinguish this accurately enough to insert in your computations. So part of this term would become indistinguishable.

PRITCHARD: Become indistinguishable from the uncertainties in the slope of the surface?

LEENDERTSE: Yes. I don't think that it is very difficult to put it in, to go to the salinity equation and compute it as a time-varying function also. I expect that it doesn't make very much difference.

PRITCHARD: I don't think that it varies very much over the tidal cycle. I think that we are talking about longer term variations.

* * *

HARLEMAN: The objectives of this third section are as follows. First, to provide a broad, critical review of the literature relating to one-dimensional models which have as their purpose some phase of a water quality problem in estuaries. Secondly, I have tried to set down the basic equations of one-dimensional continuity, momentum, and mass transfer in an unambiguous form relating to time-averaging concepts. A great deal of the emphasis here is on this problem of what period of time you are looking at when you write one-dimensional equations. (I have used the terminology in here of "real time". I am not very happy with that, and I think it probably should be changed because "real time" has certain other connotations, as most of you are aware.) Thirdly, I've attempted to clarify the nature of the assumptions made by existing mathematical models by referring back always to this concept of the period of time averaging. Fourthly, I have tried to indicate what I feel are the directions of future research and applications of one-dimensional models. I have a very strong feeling that we will still be involved with one-dimensional models for a period of time. Hopefully, we will be able to move into the more complete modeling of two- and three-dimensional problems. But this is not going to occur very rapidly, and problems that have to be handled today and tomorrow are probably going to continue to be handled in the one-dimensional framework.

The emphasis also here is on the development of predictive models, in the sense of prediction of everything except what I call water quality parameters, which are basically source and sink terms and which I feel are really the most difficult problem of water quality modeling. The real crux of the problem is the source and sink terms. For too long we have been concerned with the application of simplified hydraulic-hydrodynamic approaches which have complicated and confused the picture, and have, I think, delayed getting on with the real job of dealing with the source and sink terms and the multiple interactions that have to be considered. Certainly in these areas of interacting equations where one sink becomes a source for another term and so on, much of the important work remains to be done. These problems are so complex in defining these sources and sinks that I think this will be another reason why the one-dimensional approach will have to continue to be used. We simply don't know enough about these in even the most elementary framework to begin putting them into a more complex situation.

To summarize, then, I think that it is perfectly clear that on one-dimensional basis, if we define the geometry of an estuary, if we define the boundary conditions in terms of the tidal amplitude at the ocean and the conditions at the head of tide or whatever the upstream conditions are, and if we make some assumption about the roughness, we can then proceed to calculate the complete tidal motion without any great difficulty. We can then modify the roughness assumption by comparing these calculations with observed tidal amplitudes. Once that is achieved, we can be fairly certain that the velocities computed by this model are reasonably accurate.

So we have the technique. We have the capability of computing one-dimensional tidal motion. This, then, becomes an input to the conservation of mass equations which are discussed and shown at various places in here, for example, Equation (2.95), which I call the real time mass transfer equation. This expresses the concentration of any substance, conservative or non-conservative, in a one-dimensional variable-area estuary, in which the advective term U is the instantaneous tidal velocity that we have already calculated by solving the continuity and momentum equations.

Now we have to distinguish between the saline portion and the non-saline portion. I have not been careful here to use the word "estuary" in its precise formulation which refers only to saline regions. I consider an estuary the extent of tidal motion. Here we have to consider the part of estuaries which are non-saline or estuaries which are entirely saline, in other words in the absence of salinity gradients. By computing the tidal velocity, we can make an estimate, a fairly good one, of the longitudinal dispersion coefficient E_L based upon the work of Taylor. Now this is a very large extension of Taylor's original work.

We have done some laboratory work in oscillating flows to confirm some of these extensions, but I am not really going to argue about precise numbers of this longitudinal dispersion. I'm simply going to say that it is primarily related to the instantaneous magnitude of the tidal velocity, to the cross section, and to the roughness. The typical equation is Equation (2.127), which gives what I think is a reasonable estimate of the magnitude of E_L in the non-saline regions of estuaries. I don't really care whether this is off by a factor of two, five, or perhaps ten, because by including the instantaneous tidal velocity in the conservation of mass equation, as has already been pointed out, these longitudinal dispersion effects become much less important.

Figure 2.18 is an example of a real time solution for a continuous injection of a non-conservative substance at a point in an estuary. This is for a constant area estuary with sinusoidal tidal motion. What you see here, then, are the real time solutions shown at high water slack and at low water slack and as an average over the tidal period. The important result of this calculation is that you find concentrations existing upstream of the point of injection, roughly to a distance of 30,000 feet, primarily by virtue of the tidal motion. We then ask the question: what do we have to do to the non-tidal mathematical model for the same problem in order to replicate the real-time solution? And you see in Figure 2.23 that what you have to do is include a grossly inflated dispersion coefficient. I've plotted here solutions for 1200 ft^2/sec and 2250 ft^2/sec and neither of these is a very good representation of the real time solution. The effect of dispersion is shown relative to the real time value of 65 ft^2/sec which gives a distribution of concentration at high water slack extending again about 30,000 feet upstream, in comparison with the pseudo-dispersion of the non-tidal or slack tide models.

To summarize, what I have tried to show here is that the hydrodynamic problem, given the decay coefficient, is a simple exercise in water quality prediction. The hydrodynamic problem can be solved exactly. It can be solved in terms of an analytical solution for the constant-area estuary, and it certainly can be solved in terms of finite-difference solutions for a variable-area estuary. The real time model obviously requires more calculations. It requires knowledge of the tidal motion in the estuary, and it certainly requires that you know the geometry of the problem which you are trying to deal with. I think the basic philosophical difference between the two kinds of mathematical models devolves to this: the non-tidal model is a simple mathematical model, but it includes an arbitrary, unknown, pseudo-dispersion coefficient which hydrodynamically we cannot say anything about, because it takes up all the slack of ignoring the tidal motion. Therefore, a great deal of time and energy and effort and expense has been devoted to the determination of this type of dispersion coefficient by field tests, by dye dispersion tests, and by doing the same thing in hydraulic models (which opens up a whole new can of worms). The simplification (so-called) of a simple mathematical model then introduces a great complexity of how you find the arbitrary coefficient which this simple mathematical model introduces. So my point is that by going to a more sophisticated--and not really very sophisticated--mathematical model, one in a sense eliminates this unknown parameter, because you can make a reasonable estimate of its value. Therefore, I do not consider that we have achieved any simplification by oversimplifying the hydraulic problems. In fact, it's a great complication, to my way of thinking, because it does not really make use of present day capabilities.

I've only mentioned the dispersion in the non-saline region. There is a considerable discussion in here on how one determines the dispersion coefficient in the salinity intrusion region, and this again can be done in real time models using available data for the salinity intrusion, which is one of the most satisfactory things to measure in an estuary. The present state-of-the-art, even in terms of one-dimensional models, implies that we have to have some knowledge of the salinity distribution in order to calculate the dispersion in these areas. So what it boils down to, in terms of dispersion, is that if you are in the saline region we use the salinity measurements, and if you are in the non-saline region then we use the modified Taylor estimate.

So in summary, I would say that I think the state-of-the-art of one-dimensional modeling is such that the hydrodynamic aspects of mass transfer in estuaries should no longer be accepted as an unknown parameter, and we should stop devoting major efforts to the determination of this hydrodynamic parameter by field tests. We should get on with the much more difficult and much more important problems of making field tests which will enable us to determine the non-conservative parameters of interest in the water quality models.

RATTRAY: I'm glad to see some of your statements on this horizontal dispersion in the stratified situation, which is the one I'm more familiar with. There's a lot yet to be known about what to put in there. I think this is a fair warning.

One thing we've already mentioned is that there is a vertical shear due to the stratification, and this augments any kind of a dispersion of this kind. The other effect, that we seem to find is more noticeable maybe in the ocean, is in any stratified system the turbulent diffusion tends to be non-isotropic. That is, there will be a much larger horizontal diffusivity, without any tidal motion, than there is vertical, due to the resistance of the stratification for vertical turbulence just like for any other vertical motion. It may very well be, then, that the effects of dispersion due to shear in the vertical are not going to be dominant over horizontal diffusion in all cases. But it will be very much larger, orders of magnitude, than will be vertical diffusion. The Taylor work was done with horizontal and vertical diffusion being the same order of magnitude. I think that these are the concerns that are represented here about what happens when you go into a stratified set-up. The other limitation on this is that Taylor's work, and a lot of this here, assumes that the concentration is relatively uniform over the vertical. Not being a biologist, I would suspect many biological forms and maybe solid forms that one has to worry about in water quality do not have uniform distributions in the vertical, and that a dispersion coefficient or anything based upon a salinity distribution may be orders of magnitude off and not represent the rate of horizontal movement of those sorts of distributions.

HARLEMAN: Well, I think what you're saying is that if things aren't one-dimensional, you shouldn't use one-dimensional equations.

RATTRAY: I think we all know that, and I think you have decided that there are these limitations, and all I can do is sort of say the same thing.

HARLEMAN: If you have strong gradients in the lateral or vertical directions, then you shouldn't expect to get good results from one-dimensional equations.

PRITCHARD: Well, I might say that I've been sort of a reluctant admirer of the success of the one-dimensional equations, both the dynamic equation and what you might call the mass balance equations or salt balance equations, even in systems which I always thought had some variation across the cross section. I don't want to belabor the point too long but I think it's of interest to try to decide why certain integrals disappear. That is, if I take the three-dimensional equation of motion and salt continuity and integrate them over the cross-section, I can get forms that look exactly like the forms that Don has shown here, plus some additional terms, the additional terms being terms which involve the cross product of the velocity deviation terms in the cross section referred to the cross-sectional means. In the salt balance (or the mass continuity equation, the conservation of a substance) there also appear some of these additional terms, which involve the cross product of the deviation in the velocity times the deviation in the salinity from their sectional means. Where the system is reasonably homogeneous, these terms are probably small, but where there is a shear, either laterally or horizontally, the deviation in the horizontal velocity with position in the cross section and the deviation in the salinity with position in the cross section from their respective cross-sectional means must be highly correlated, so that these cross products must really be real fluxes. It's amazed me that in estuaries like the Delaware one appears to be able to treat it as one-dimensional. I guess it must be that even though the fluxes may be large, the gradients must be small. It's just phenomenal. As I say, I've been a reluctant admirer of its success. I would just point out that I think that people using these relationships certainly must not jump too readily to the conclusion that a one-dimensional situation is going to work everywhere. And I think this has been said.

RATTRAY: On this one-dimensional model in general, this thing has sort of been raised again. It is quite evident, to me, that no purely advective model will give any dispersion. There has to be some diffusive term in there. That's true even if you include turbulence, that is, you wouldn't have diffusion by turbulence unless there was molecular diffusivity working also. The reason you normally can neglect the molecular diffusivity part is that you're working in large Reynolds numbers, so that there is a lot of energy in the turbulence and there is a very small transfer being done by molecular processes. The turbulence is in very large gradients for very rapid diffusion by molecular processes. This same thing has to be going on when you use tidal motion. It must give you large gradients which are diffused by something in the model or you would never have a one-dimensional model with any diffusion at all.

PRITCHARD: There has to be diffusion by the turbulence, diffusion which in turn then really goes back to molecular. If you follow the theory all the way, you would have to include in the physical description molecular diffusion or molecular viscosity.

RATTRAY: But I would like to make the further analogy that the thing that would be important, then, is that the tidal terms themselves would give the major part of the diffusion if the effective Reynolds number were large. It would be independent of the turbulent terms for large Reynolds number type behavior. But if you have the case where the effective Reynolds number, using a turbulent eddy diffusivity, is not large, then of course it starts to depend upon the eddy turbulent diffusivity, just like if in turbulent flow you go towards the molecular limit. You can get to the point where both diffusions are significant. This has to be worried about. Apparently in most cases we don't reach that, just judging by the success. Maybe you don't even have to put it in. Maybe you get enough turbulence in roundoff errors in a numerical model. But it has to be there. It shouldn't be forgotten that it's there somehow.

THOMANN: On use of tidal models with tidal variability in the velocity term (and it's fairly large in most of these estuaries), there really is a question, for example, in some of your plots that are shown here, Dr. Harleman, about whether there would really be any difference between those and what you would have if you had set that dispersion coefficient to zero.

HARLEMAN: However, when you use finite-difference forms that's a more difficult problem. We want some dispersion in the model.

THOMANN: Why?

RATTRAY: You need it.

THOMANN: Why? Actually you'll introduce some right off the bat in a finite-difference model, and that may be more than you need.

HARLEMAN: You don't have to worry about that. If you are going to have a continuous model that goes from the non-saline region to the saline region, you want to have some mechanism for introducing dispersion. So if you are going to have dispersion in the salinity region, which you definitely need, then there's no reason why you shouldn't include it in the non-saline region.

THOMANN: Yes, but all I am pointing out is that it may be quite insensitive.

HARLEMAN: Well, that's what I am saying.

THOMANN: But where it does become important, and one can show this, is when the input at the boundary is fluctuating with a certain frequency, and then one has to be very careful about incorporating even small amounts of dispersion, and the difference between the straight advective model and the dispersive model can be quite large. But in the analysis that Dr. Harleman presents, would those profiles be substantially different if E, which is about 60 ft^2/sec, were set at zero?

PRITCHARD: It would not be very different in the numerical output, but remember you've got dispersion in the numerical equation.

THOMANN: Yes, right. And all I am saying is that when you incorporate the tidal velocity as a time variable in the equation, for many practical purposes the inclusion of the dispersion coefficient E may be unnecessary.

HARLEMAN: Unless you get into the salinity gradient.

THOMANN: Yes.

HARLEMAN: But if you are going to include it in the salinity region, then there is no reason not to include it in the non-saline region even though it's small.

PRITCHARD: Do I understand you, that when you move into the salinity region or into the region in an estuary where the salinity gradients are high, that E_L term, even with the real time system, becomes larger than the Taylor E_L ?

HARLEMAN: Yes, it becomes quite large, and quite a function of x .

PRITCHARD: And even larger if you average over the tide. But even if you don't average over the tide, if you use a real time solution, you still have an E_L which you've got to relate to something else besides the Taylor equation.

HARLEMAN: We are relating it now to the local salinity.

PRITCHARD: Right. But if you go back to your flume work, you related it to the difference in the salinity of the river input and the ocean. If you go to some of those relationships, you come up with the pertinent factor involving the ratio of a Froude-type number and a velocity at the surface to the tidal velocity relationship.

RATTRAY: Well, again I come back to the fact that you have to have two parameters and that the salinity differences do not give you the velocity profiles uniquely. It's the velocity profiles that cause the dispersion and not the salinity differences.

HARLEMAN: We're only talking about one-dimensional models so we can't include velocity profiles. The momentum and continuity equations give you the tidal velocities.

RATTRAY: Well, in terms of the dispersion coefficient, the salinity profile in the saline region must be very important, and I think you've said that. But the way of getting at it is more complicated.

HARLEMAN: The way of getting at it is to simply take the measured salinity and match it, in a one-dimensional framework. Then you have included everything that is there in the one-dimensional model, because you have matched the existing salinity distribution.

PRITCHARD: I think where we would have a problem is if we intended to predict everything from the boundary values and the hydrodynamics, that is, including the salinity distribution. Then we want to have some independent way of estimating these things in order to compute the salinity, as well as the distribution of properties. As you say, for many practical problems, in the near future reduced-dimensional models may still be desirable. Hence we would like to get at ways to independently predict the terms that enter some of these averaged equations, even recognizing the fact that it is not truly one-dimensional or two-dimensional.

HARLEMAN: Well, this section of Chapter II does include some discussion of predicting salinity intrusion changes on a one-dimensional basis, which is a requirement for what you say.

PRITCHARD: Yes, that's what I'm getting at. The results of some of your flume studies which you then apply to the Delaware. And as I say, the success of that has been remarkable.

DOBBINS: I think there is one other question I'd like to raise here. In these steady-state models, if you determine a value of E based on longitudinal salinity distribution, if you make a dye dump, say, an instantaneous dump, and determine E, and if you, let's say, determine E for a continuous dump, are you going to get the same value? I don't think you are. And therefore it is not valid to measure E from a salinity distribution and apply that to determine the fate of a pollutant. I don't think this is being recognized in many cases. That is, everybody thinks it's the same E, but it isn't.

HARLEMAN: They are not the same initially, but they approach each other rather quickly in time.

PRITCHARD: You mean as the scales of the phenomena get to be identical?

HARLEMAN: If you were concerned with an instantaneous release, this difference would be quite large; but not if you are concerned with continuous releases.

DOBBINS: Most of the dye dumps that are made are, after all, instantaneous releases.

HARLEMAN: But I'm saying we shouldn't make them, because it isn't what we want to solve. If you are interested in solving the problem of the dye dump, okay. But why do a dye dump to solve some other problem?

DOBBINS: Well, that's my point.

RATTRAY: The point is, isn't it, that in many cases you are using a mean salinity to solve other problems. It's not valid.

DOBBINS: Right. Also, I think this is a question of whether you're interested in local effects. Take, for example, the city of Poughkeepsie, which takes its water supply out of the Hudson River just about the head of the tide. You are going to be very, very much concerned about the diurnal variation of the water quality there. In fact they've run into severe problems of treating this water because of the diurnal variation in the quality.

PRITCHARD: I should bring in a future paper which shows a comparison between a distribution of temperature from a thermal discharge averaged across a section as computed from coefficients gotten from the salinity distribution, and show you the comparison with the real distribution. They are very close. I am now talking about scales which are clear across the estuary, averaged in a section. This was an input which essentially was not local, and it worked.

CHAPTER III

WATER QUALITY MODELS:
CHEMICAL, PHYSICAL AND BIOLOGICAL CONSTITUENTS

Donald J. O'Connor
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1. INTRODUCTION

Any natural body of water may be viewed as a mathematical system, composed of a number of complex interacting subsystems. The system receives, on the one hand, a series of external inputs such as rainfall, solar radiation, runoff, and winds which determine the natural quality of the water. On the other hand, the system is also subjected to a variety of man-made inputs such as wastewater discharges, water diversions, runoff from urban and land developments. The response of the system to each of these inputs is the spatial and temporal distribution of the concentration of various substances which affect water use. Such substances include various chemicals, dissolved oxygen, nutrients (nitrogen and phosphorous), bacteria and algae concentrations, and dissolved and suspended solids. The system is composed of a number of parts, with physical characteristics and corresponding mathematical descriptions. Physically, the concentration of these substances is determined by the dispersion and advection characteristics of the water body and by the various physical, chemical, biological or radiological reactions which affect the substance. Mathematically, the system is described by a set of partial differential equations, with variable coefficients, each term of which corresponds to one of the basic characteristics. Modifications of these equations comprise a water quality mathematical model.

The purpose of a model of any system is to reproduce in some way the observable phenomena which are of particular significance. From a scientific viewpoint a model provides greater understanding and insight of the phenomena, and from an engineering perspective it provides a means of prediction and, therefore, control of the system. In both cases, there is posed a specific question or problem to which the construction of the model is directed. Fundamental to the development are the time and space scales of the phenomena involved and/or the question posed, which, to a large extent, determine the nature and complexity of the model.

Relating these concepts to the modeling of water quality in natural systems, three criteria may be applied which determine the nature and characteristics of the model.

(1) The water quality problem. The time scale of the problem is the most important element which determines the type of model to be employed. In this respect it is frequently possible to isolate a singular scale within which the analytical framework of the solution may be structured. For example, is the problem concerned with the relatively short-term variation

of water quality, due to, for example, a storm water overflow in an estuary, or with the long-term accumulation of a conservative material in a tidal bay or harbor? In the first case, the time scale is in the order of hours or days, while in the latter, it may be of years or decades.

(2) The characteristics of the water body. Each body of water is characterized by its own geomorphological structure and a set of hydrological-meteorological inputs which determine to a large extent the hydrodynamic regime of the system. Each regime has its own characteristic scale in both time and space. In the case of estuaries, a most predominant time scale from the hydrodynamic point of view is the tidal period, and, therefore, may be an important factor to include in water quality modeling. However, it is not necessarily a significant factor. Referring to the example above, it is significant in the case of the storm water overflow where the time scales are of the same order. Since it is necessary to account for hour-to-hour variation in water quality, it is obvious that the hour-to-hour variation in the tides must be included. On the other hand, if the accumulation of a pollutional material in a tidal bay is in the order of years, the hour-to-hour variation in the tides may not be significant and may frequently be neglected without introducing significant error.

(3) The reaction time of the pollutants. This factor is determined largely by the nature of the substance and the physical, chemical and biological reactions to which it responds. In similar fashion to that described above, the time scale can range from very short, almost instantaneous reactions to those which persist for such long periods that the substances affected may be regarded as conservative. Again, there may be a spectrum of time scales for a particular parameter. For example, one may be interested in modeling algae dynamics for a short-term bloom over a period measured in hours or days, or over the year in which the seasonal variations are apparent and the time scale is in the order of weeks, or over a eutrophication period of decades for which the scale would be based on units of a year. Relating the scale of these phenomena to the hydrodynamic scales, the tidal variations are the most significant in the short-term bloom. In the seasonal variation of algae, the hydrologic factors such as the freshwater flow and the temperature assume primary importance, while the tidal effects, although significant, may be incorporated in a relatively simplistic manner. In the long-term buildup, the tidal factors are even less significant, while the year-to-year water balance, as directed by long-range weather patterns, is the most influential hydrodynamic factor.

Fundamental to the analysis of the problem is the continuity equation. The point form of this equation is

$$\frac{\partial c}{\partial t} = \nabla \cdot j \pm \Sigma S \qquad (3.1)$$

in which

c = concentration of water quality variable
t = time in tidal cycles
S = sources and sinks of variable c
j = flux = $E \frac{\partial c}{\partial n} - Uc$
E = tidal dispersion coefficient
U = freshwater flow velocity

The continuity equation expresses a relationship between the flux of mass and the sources and sinks of mass where the flux of mass is considered to occur from tidal cycle to tidal cycle.

For within-tidal-cycle descriptions, the velocity U is interpreted as the tidal velocity (see Chapter II). The term Uc is the flux due to advection by the fluid containing the mass. The term $E\ \partial c/\partial n$ is the flux commonly ascribed to dispersion in the "n" direction. The flux due to dispersion is assumed to be proportional to the gradient of concentration in the direction of decreasing concentration. Any mass of pollutional substance is transferred by this mechanism from a zone of high concentration to one of low concentration. The flux is determined by the hydrodynamics of the system, which is related to the hydrology, meteorology and geomorphology of the areas. The sources and sinks are the results of the various reactions of a physical, chemical or biological nature. Many factors contribute to the total spread of mass, and the term tidal dispersion rather than diffusion more appropriately describes the phenomenon. The coefficient E includes not only the diffusion associated with turbulent mixing but also the dispersion due to velocity gradients and density differences (Harleman 1964). As such, this coefficient incorporates the major features of the tidal mixing phenomena in estuaries and provides a useful approximation for many water quality studies. The relative advantages and disadvantages of finer time scaling of the model to describe hour-to-hour changes in some water quality variables have been discussed (Callaway et al. 1969 and Chapter II, Section 3 of this report). Generally the trade-off involves longer computer time versus introduction of the inter-tidal dispersion coefficient. In particular, the dispersion factor is affected in streams by freshwater flow, in estuaries by the tidal translation and the freshwater flow, and in the oceans by the various currents. The velocity coefficient U is likewise determined by many of these parameters. These hydrodynamic coefficients, as well as the source term S, may be both time and space variables.

While the flux term defines the material moving in and out of an elemental volume, the term ΣS represents the sum of the various sources and sinks of material within the volume. Characteristic sources and sinks are reactions of a physical, chemical or biological nature which occur in natural waters. Many of these reactions may be represented by first-order kinetics, i.e. the rate of the reaction is proportional to the concentration of the substance. The coefficient K, which is the proportionality constant in the first-order reaction, is characteristic of many reactions in water pollution. In some cases it fundamentally defines the mechanism, as in the case of radioactive decay or gas transfer; in other cases it is an empirical approximation of the phenomenon, e.g. the decay of waste material and the bacterial die-away.

The three dimensional form of Equation (3.1) is

$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial x}\left(E_x \frac{\partial c}{\partial x}\right) + \frac{\partial}{\partial y}\left(E_y \frac{\partial c}{\partial y}\right) + \frac{\partial}{\partial z}\left(E_z \frac{\partial c}{\partial z}\right)$$

$$- \frac{\partial}{\partial x}(uc) - \frac{\partial}{\partial y}(vc) - \frac{\partial}{\partial z}(wc) \pm \Sigma S \qquad (3.2)$$

in which the subscripted E refers to the dispersion coefficient along each of the three axes. Equation (3.2) may be simplified to steady state in many cases, particularly at that period of year when the freshwater flow and temperature are approximately constant and the waste water discharges may be assumed so. The analysis of some estuaries is further simplified by virtue of the fact that the concentration of various substances over the cross-sectional area has been observed to be uniform, thus reducing the problem to one dimension. It is the steady-state one-dimensional form of Equation (3.2) which has found the most extensive application in the analysis of estuarine pollution.

Longitudinal tidal dispersion is most important in the saline portion of the estuary where a number of factors contribute to the intrusion of the salt into the estuary (see Chapter II). The concentration of other substances which are of concern in water quality in estuaries is affected in a manner similar to that of the salt. In the tidal but nonsaline sections of the river, the dispersion although not as pronounced as in the saline section is still a significant factor in the analysis of water quality. Upstream of the tidal influence, the effect of longitudinal mixing is much less and in many cases may be disregarded, depending on the relative magnitude of the dispersion, advection and reaction.

As previously indicated, the sources and sinks refer to the various reactions and waste water inputs which affect the concentration of material in the estuary. In terms of the pertinent water quality variables, at one end are the conservative (no decay) substances such as the chloride concentration, and at the other end such quantities as dissolved oxygen, various nitrogen forms and phytoplankton, which are the result of a series of coupled reactions. It is convenient to first consider material which is conservative, secondly a single decaying species, followed by a consecutive two-stage reaction, and lastly a multi-stage reaction.

2. ONE-DIMENSIONAL ANALYSIS

The form of Equation (3.2) which is appropriate for the one-dimensional analysis in estuaries is (O'Connor 1960 and 1965)

$$\frac{\partial c}{\partial t} = \frac{1}{A} \frac{\partial}{\partial x} \left(EA \frac{\partial c}{\partial x} \right) - \frac{1}{A} \frac{\partial}{\partial x} (QC) - Kc \qquad (3.3)$$

where A is the cross-sectional area of the estuary, Q is the freshwater inflow and K is the first-order decay coefficient. This equation is the one-dimensional estuarine model for the dispersion and advection of a non-conservative substance subjected to a first-order reaction. It should be noted again that this equation is assumed to apply over a time interval of at least a tidal cycle. Many substances of practical interest are susceptible to physical, chemical or biological decay of this type including coliform bacteria and biochemical oxygen demand. In those cases in which the substance is conservative, the solutions for the non-conservative case usually hold with $K = 0$. Although the diminution of concentration may be effected by many different mechanisms and factors, the assignment of a first-order reaction is most appropriate and practical, from both theoretical considerations and experimental observations. Most of the common pollutants are subject to a decay of this order. However, as discussed in Section 7 of this chapter, complex nonlinear reaction kinetics can be incorporated in the more advanced models of algal productivity.

In general, the solution to an instantaneous waste discharge (a delta function input) provides the key to the solution of the transient and the steady-state conditions, all three of which have practical value. The delta function input, which is referred to as $\delta(t)$, is that of an instantaneous release of mass M uniformly distributed over the cross-sectional area A at the origin $x = 0$. By integrating the solution of Equation (3.3) with a delta function input with respect to time, the solution of the continuous source is obtained. If the discharge is given at a rate $W(t)$, starting at time $t = 0$ and continuing to time t, then the following equation gives the concentration $c(x,t)$ at time t and location x:

$$c(x,t) = \int_0^t W(t') \, c_\delta (t - t') dt' \qquad (3.4)$$

where $c_\delta (t - t')$ is the solution of Equation (3.3) due to the instantaneous input. If $W(t)$ is constant, the expression is simplified and the solution for the steady state for this condition is

$$c_{(x,\infty)} = \int_0^\infty c_\delta (t - t') dt' \qquad (3.5)$$

Alternately the steady-state solution may be determined from the original equation (3.3) by letting $\frac{\partial c}{\partial t} = 0$ and seeking a solution of the ordinary differential equation. Solutions of various spatial distributions are similarly found by integration of the appropriate equation with respect to distance. In principle, any type of spatial or temporal input of a waste water source may be formally evaluated if the solution to the delta function is available.

2.1 SOLUTION DUE TO INSTANTANEOUS RELEASE

Consider an estuary of constant cross-sectional area and constant flow. For a non-conservative substance, Equation (3.3) simplifies to

$$\frac{\partial c}{\partial t} = E\frac{\partial^2 c}{\partial x^2} - U\frac{\partial c}{\partial x} - Kc \tag{3.6}$$

in which the longitudinal tidal dispersion E, the velocity U, and the reaction K, are constants. If a mass of material is released instantaneously at time $t = 0$ and uniformly over a cross section whose location is designated as the origin, then the solution of Equation (3.6) is

$$c = \frac{M}{2A\sqrt{\pi E t}}\exp\left(\frac{-(x-Ut)^2}{4Et} - Kt\right) \tag{3.7}$$

The mass M is released at $t = 0$ over the area A, located at $x = 0$. As the material moves downstream its concentration is decreased by the characteristic reaction and its mass is spread upstream and downstream from its center of gravity, which moves at the net downstream velocity of the estuary.

Since Equation (3.7) has the same mathematical form as the normal or Gaussian probability density function, it may be seen that the spatial distributions are symmetrical for a specific tidal cycle. The peak concentrations of the spatial distributions occur at $x = Ut$ and the dispersion about the peak may be described by

$$c = c_o\exp\left(\frac{-x_p^2}{4Et}\right)$$

or (3.8)

$$c = c_p\exp\left(\frac{-x_p^2}{4Et}\right)$$

in which

$c_o = \frac{M}{2A\sqrt{\pi E t}}$ = peak concentration at time t of a conservative substance

$c_p = c_o\exp(-Kt)$ = peak concentration at time t of the non-conservative substance

x_p = distance measured from the peak concentration

These equations may be used to describe the spatial distribution about a point which moves with the mean velocity of flow.

The temporal distribution, on the other hand, for a fixed point in space is asymmetrical and the degree of skewness depends upon the magnitude of Ut as compared to $(4Et)^{\frac{1}{2}}$. The spatial and temporal distributions of the delta function solution are shown in Figure 3.1.

If a substance in solution or suspension is released continuously, its concentration will increase in time at a fixed location until an equilibrium value is achieved, as shown in Figure 3.2. The manner in which this increase occurs for a conservative substance may be

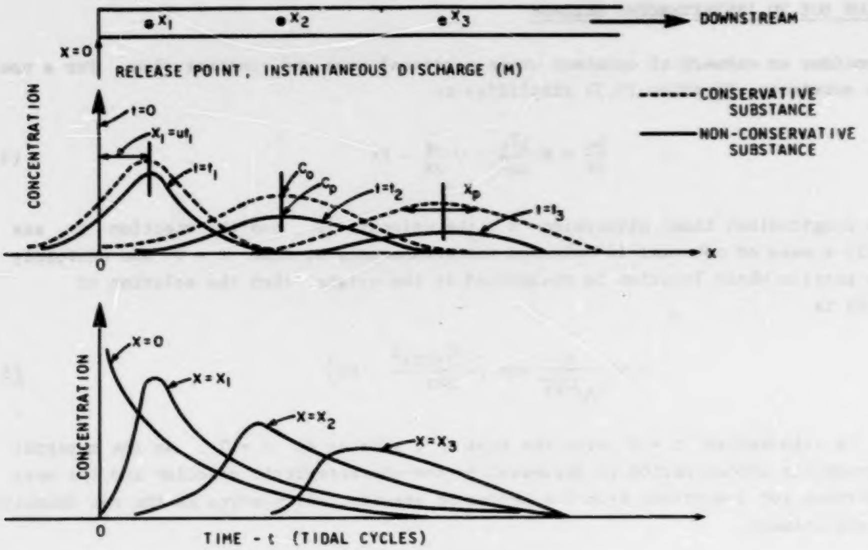

x₁
x₂
x₃
DOWNSTREAM
x=0
RELEASE POINT, INSTANTANEOUS DISCHARGE (M)
CONSERVATIVE SUBSTANCE
NON-CONSERVATIVE SUBSTANCE
CONCENTRATION
t=0
x₁=ut₁
t=t₁
C₀
Cp
t=t₂
xp
t=t₃
x
0
CONCENTRATION
x=0
x=x₁
x=x₂
x=x₃
0
TIME - t (TIDAL CYCLES)

Fig. 3.1 **Temporal and spatial distributions of water quality due to instantaneous discharge.**

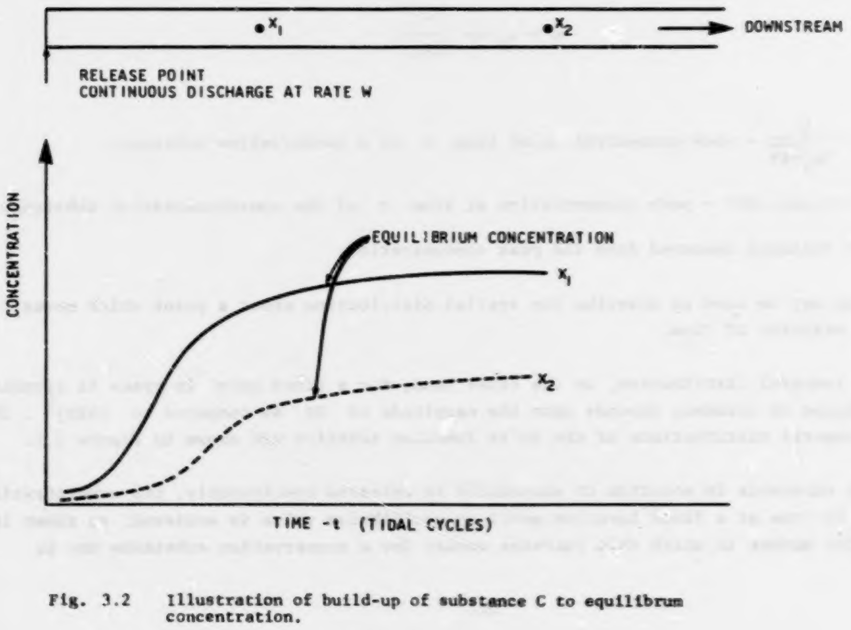

x₁
x₂
DOWNSTREAM
RELEASE POINT
CONTINUOUS DISCHARGE AT RATE W
CONCENTRATION
EQUILIBRIUM CONCENTRATION
x₁
x₂
TIME -t (TIDAL CYCLES)

Fig. 3.2 Illustration of build-up of substance C to equilibrum concentration.

determined at a particular station by the operation indicated in Equation (3.4). The resulting expressions are not always directly integrable and arithmetic integrations are frequently required. In effect, this build-up time to an equilibrium depends on the interaction between the tidal dispersion phenomena, freshwater flow and reaction coefficient. For rivers where E approaches zero, time to reach equilibrium is almost instantaneous. For estuaries, equilibrium times may be on the order of days or weeks.

2.2 CONSERVATIVE SUBSTANCES

The saline intrusion of the ocean waters into the river provides a classic example of a conservative substance in an estuarine system. For some problems, it is useful to consider other variables such as the total nitrogen or total phosphorous to also be conservative. In these cases, overall mass balances between waste water inputs and land runoff can be analyzed. Waste waters from various sources may contain substances not indigenous to the natural runoff. Such substances (e.g., sulfates) may act as tracers of such sources, since their concentration is easily detectable by contrast to the amount present from natural sources.

The form of Equation (3.3) which is appropriate for conservative substances under the steady state is

$$0 = \frac{1}{A}\frac{d}{dx}\left(EA\frac{dc}{dx}\right) - \frac{1}{A}\frac{d}{dx}(Qc) \qquad (3.9)$$

Integration once and application of the appropriate boundary condition yields, without loss of generality concerning the spatial variation of the parameters,

$$0 = \frac{dc}{c} - \frac{Q}{EA}\,dx \qquad (3.10)$$

which upon integration gives

$$c = c_o \exp\left[\int \frac{Q}{AE}\,dx\right] \qquad (3.11)$$

The boundary condition c_o at $x = 0$ may apply in practical cases to a point where the concentration is known or may be established, e.g. at the mouth of the river for the saline intrusion analysis or at the location of a waste water source of a conservative substance. In either case, and in many other practical situations, the concentration in the ground water is insignificant by contrast to the concentration in the tidal river and may be usually neglected. Constant values of Q , A and E characterize the simplest tidal river and provide a model which may be used as an approximation of prototype conditions. The differential equation for constant parameters is

$$0 = E\frac{d^2c}{dx^2} - U\frac{dc}{dx} \qquad (3.12)$$

and its solution, which may also be written directly from Equation (3.11) is

$$c = c_o \exp(jx) \qquad (3.13)$$

where $j = \frac{Q}{AE}$

A common application of Equation (3.13) is made in the evaluation of the dispersion coefficient E from observations of the salinity or chloride concentration in estuaries. In this application, a semi-log plot of chloride concentration with distance is prepared. According to Equation (3.13), the slope of a straight line through these data is given by Q/AE from which E can be obtained. Typical values of this overall tidal dispersion coefficient for estuaries range from 1-15 square miles/day in the non-saline sections and 5-25 square miles/day in the saline.

In many cases, the parameters Q , A and E , and particularly the latter two, vary with distance. Various functional forms may be substituted in Equation (3.11) and integrated. Alternately the estuary may be segmented as discussed in subsequent sections.

2.3 NON-CONSERVATIVE SUBSTANCES

In the steady state and for constant coefficients, Equation (3.3) reduces to

$$0 = E\frac{d^2c}{dx^2} - U\frac{dc}{dx} - Kc \tag{3.14}$$

The form of the general solution of this ordinary differential equation is

$$c = B\exp(gx) + C\exp(jx) \tag{3.15}$$

in which

$$g = \frac{U}{2E}\left[1 + \sqrt{1 + \frac{4KE}{U^2}}\right]$$

$$j = \frac{U}{2E}\left[1 - \sqrt{1 + \frac{4KE}{U^2}}\right]$$

B and C are constants to be evaluated from the boundary conditions. The exponents are the positive and negative roots of the quadratic expression which contains the coefficients of the differential equation, E , U and K . It is readily shown that for an infinitely long estuary into which a pollutant is being discharged at a constant rate, the solution may be generally expressed as

$$c = c_o\exp(gx) \text{ for } x < o \tag{3.16a}$$

$$c = c_o\exp(jx) \text{ for } x > o \tag{3.16b}$$

Equation (3.16a) applies to the region upstream of the discharge and Equation (3.16b) to the downstream section (positive x in the downstream direction). The concentration c_o and the exponents g and j take on particular values, depending on the magnitudes of E , U and K . If these parameters are greater than zero, it can be shown that

$$c_o = \frac{W}{A\sqrt{U^2 + 4KE}} = \frac{W}{Qm} \tag{3.17}$$

where

$$m = \sqrt{1 + \frac{4KE}{U^2}}$$

These expressions apply to the distribution of a non-conservative substance in a river with significant dispersion and freshwater flow. If a conservative substance is considered the expressions become

$$c_o = \frac{W}{AU} = \frac{W}{Q}$$

$$g = \frac{U}{E} \tag{3.18}$$

$$j = 0$$

It is apparent that the concentration downstream from the outfall is constant, since $j = 0$. The concentration upstream, however, decreases due to the back dispersion which balances the advective component downstream.

If the freshwater flows are zero, the advective component drops from the basic equation and the expressions become

$$c_o = \frac{W}{A\sqrt{4KE}}$$

$$g = j = \sqrt{\frac{K}{E}} \tag{3.19}$$

Since the exponents are equal, it is apparent that the upstream and downstream distributions are symmetrical about the discharge point.

If the dispersion coefficient is zero and the advective component greater than zero, the basic differential equation simplifies to a first-order form and represents the non-dispersive case that is often used in nontidal rivers and streams. The solution for the concentration is

$$c = c_o \exp\left(\frac{-Kx}{u}\right) \tag{3.20}$$

where

$$c_o = \frac{W}{Q}$$

which can be recognized as the equation used to describe the BOD in streams. The significant dimensionless number is $P = KE/U^2$. One limit, $P = \infty$ is characteristic of highly dispersive or estuarine systems; more specifically, a system in which the dispersion is so great by contrast to the advection that the latter may be neglected. The other end of the spectrum, where $P = 0$, represents strictly advective systems, as characterized by freshwater streams, in which the reverse is true. As one moves downstream from the freshwater sections through the deep river stretches and thence to the tidal portions and finally to the saline outlet at the ocean, the value of "m" in Equation (3.17) increases.

The importance of the reaction coefficient must not be overlooked in the structuring of the model. From the physical or hydrodynamic point of view, it is the ratio of the dispersion and advection which determines the most realistic model. From a chemical or biological point of view, it is the magnitude of the reaction coefficient which is the determining factor. For many estuarine situations, the water quality response tends to be more sensitive to the reaction coefficient than to the tidal dispersion coefficient.

2.4 CONSECUTIVE REACTIONS (BOD-DO)

A common example of a consecutive reaction is the dissolved oxygen deficit produced by the concentration of oxygen-demanding material through biological action or chemical oxidation. Under the steady-state constant-coefficient condition, the differential equations for concentration of the two reactants are

$$0 = E\frac{d^2c_1}{dx^2} - U\frac{dc_1}{dx} - K_{11}c_1 \qquad (3.21)$$

$$0 = E\frac{d^2c_2}{dx^2} - U\frac{dc_2}{dx} - K_{22}c_2 + K_{12}c_1 \qquad (3.22)$$

where K_{11} is the decay coefficient associated with the concentration c_1 and acts as a sink in a typical first-order decay phenomenon, K_{12} is a reaction coefficient and together with c_1 acts as a source for c_2, and K_{22} is the decay coefficient associated with variable c_2. For continuity, $K_{11} \geq K_{1j}$. For the case of dissolved oxygen, c_1 represents the carbonaceous or nitrogenous BOD, K_{11} represents the BOD decay rate (which may include oxidation and settling), K_{12} is the deoxygenation coefficient, K_{22} is the reaeration rate, and c_2 is the dissolved oxygen deficit. The solution of Equation (3.21) is shown by Equations (3.16a) and (3.16b) for a single discharge of waste water W_1 (mass/unit time). Substitution of these equations into (3.22) yields an expression for the concentration of the second reactant. Substitutions are made for both the negative and positive values of x, i.e. both Equations (3.16a) and (3.16b). The solution of Equation (3.22) given Equation (3.16a) and (3.16b) as input is

$$c_2 = \frac{K_{12}}{K_{22} - K_{11}}\left(\frac{\exp(j_{11}x)}{m_{11}} - \frac{\exp(j_{22}x)}{m_{22}}\right)\frac{W}{Q} \qquad (3.23)$$

where

$$j_{11} = \frac{U}{2E}\left[1 - \sqrt{1 + 4K_{11}E/U^2}\right]$$

$$j_{22} = \frac{U}{2E}\left[1 - \sqrt{1 + 4K_{22}E/U^2}\right]$$

$$m_{11} = \sqrt{1 + 4K_{11}\,E/U^2}$$

$$m_{22} = \sqrt{1 + 4K_{22}\,E/U^2}$$

for $x > 0$. For $x < 0$, replace j_{11} and j_{22} with g_{11} and g_{22} as per Equation (3.16a). Note that for this coupled system the reaction coefficients of the equations act as multipliers in the solution.

The coordinates of the maximum value c_{2_m} are obtained as follows. The distance x_m to the maximum value of c_2 is evaluated by differentiating Equation (3.23) and setting the result equal to zero. After simplification, the distance is

$$x_m = \frac{1}{j_{11} - j_{22}} \ln\left(\frac{m_{11}\,j_{22}}{m_{22}\,j_{11}}\right) \tag{3.24}$$

The value of the maximum c_{2_m} may be determined by substituting Equation (3.24) in Equation (3.23); or, alternatively, by taking the second derivative of Equation (3.23), substituting in Equation (3.22), setting the first derivative term equal to zero and evaluating the result. The expression for the maximum value of c_2 is

$$\frac{C_{2m}}{L_o} = \frac{1}{\alpha_k - 1}\left(1 - \frac{1}{\alpha_j}\right) \exp\left(\frac{1}{1 - \alpha_j} \ln \frac{\alpha_j}{\alpha_n}\right) \tag{3.25}$$

where $\alpha_k = K_{22}/K_{11}$, $\alpha_m = \sqrt{1 + 4\alpha_k K_{11}E/U^2} \Big/ \sqrt{1 + 4K_{11}E/U^2}$,

and $\alpha_j = \left(1 - \sqrt{1 + 4\alpha_k K_{11}E/U^2}\right) \Big/ \left(1 - \sqrt{1 + 4K_{11}E/U^2}\right)$.

2.5 APPLICATIONS TO DISSOLVED OXYGEN ANALYSIS

Equation (3.23) merits particular attention in view of its wide application in the analysis of water quality data. The most significant example of its application is in the analysis of the spatial distribution of the concentration of dissolved oxygen in tidal rivers and estuaries. Graphical presentations of Equation (3.16) and Equation (3.23) are shown in Figure 3.3. The former represents the concentration of a substance which utilizes oxygen, such as the respiration of bacteria or algae, the biochemical oxygen demand (BOD) or a chemical oxidation. The mass rate of discharge is indicated by W and the freshwater flow by Q . The latter equation describes the distribution of dissolved oxygen deficit due to the concentration of the former. The coefficient of oxidation or deaeration is identified by the symbol K_{12} and the reaeration by K_{22} . The solid line represents the mean tide of the ebb or flood, while the dotted and dashed lines are the profiles at ebb and flood slack, respectively.

The primary purpose of such an analysis is to assess the effect of waste waters on the dissolved oxygen levels and, in particular, to determine the efficacy of various engineering

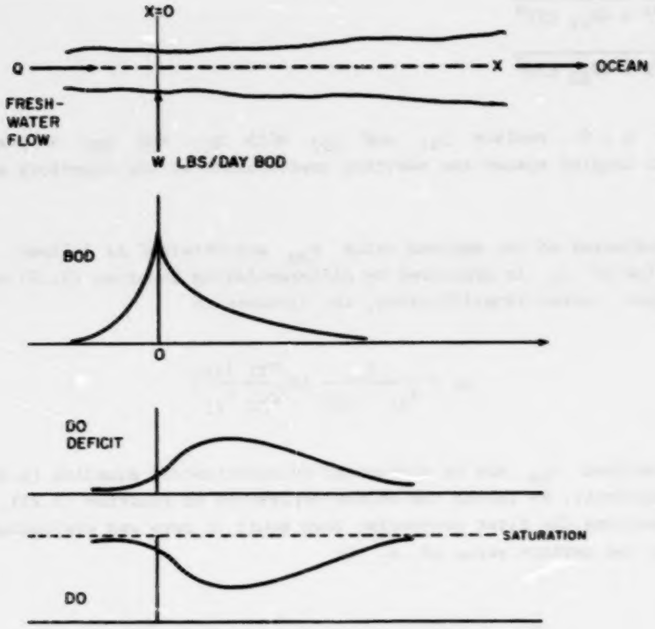


Fig. 3.3 Estuarine BOD, deficit and DO profiles.

alternates in restoring water quality or in preventing deterioration of quality. On the one hand, the analysis is used to predict dissolved oxygen levels given degrees of treatment for the various waste constituents. On the other hand, the analysis may be used to determine the degree of treatment required of the various waste constituents to restore or maintain water quality of appropriate levels.

The information required for such an analysis may be divided into the following categories. The assumption of the steady-state condition is frequently valid if the waste discharge is constant during the low-flow, high-temperature period of the late summer and early fall.

(1) Waste Water Discharges. It is necessary to know the nature and quantity of the various constituents of waste waters which use dissolved oxygen. It is the oxidation of these substances, either biologically or chemically, which causes a depression of the oxygen levels in estuaries. Most waste may be divided into carbonaceous and nitrogenous components, each of which biochemically utilize dissolved oxygen at different rates. Furthermore, the suspended and dissolved fraction of each component of each waste should be assessed. The former fraction may be susceptible to settling, producing typical benthal deposits and sludge banks which cause an additional claim on the oxygen resources. Some industrial wastes contain components which may be oxidized chemically such as the ferrous or the sulfite ion. The nitrogen part of wastes may be oxidized biochemically by nitrifying bacteria or assimilated by phytoplankton, which in turn use dissolved oxygen in their respiratory processes.

(2) Physical, Chemical and Biological Reactions. The waste discharges, described above, act as sinks of dissolved oxygen insofar as the various constituents of these wastes are oxidized in estuarine environment. The rates at which these reactions progress are essential to the analysis. They are functions of the characteristics of the biophysical environment. Temperature is usually the most predominant factor, although sunlight, winds, velocity and the nature of the estuarine channel, among others, may also be factors. The reactions are influenced by the chemical or biological nature of the constitutent, by its carbon, nitrogen, and other components, and by the state of solution or suspension. Each factor affects the dissolved oxygen in its own fashion and should be evaluated separately. In general, each type of waste--municipal, industrial, agricultural and natural--should be broken down into the following categories for dissolved oxygen sinks:

1. Carbonaceous component
2. Nitrogenous component
3. Potential for sludge deposits
4. Chemical oxidation
5. Algae respiration

In addition to the reactions which cause the depletion of oxygen, account must be taken of those reactions which act as sources of oxygen, such as atmospheric aeration, photosynthetic production and anaerobic reduction. Each of these are also functions of temperature and other biophysical conditions. The specification of the reactions, which act as either sources or sinks of dissolved oxygen, is a most critical step in the modeling effort.

(3) Hydrodynamic Factors. While the reactions described above determine the increase or decrease of dissolved oxygen within a segment of the estuary, the hydrodynamic factors fix the transport of oxygen in and out of the element. The flux consists of dispersive and advective factors due to tidal phenomena, circulation and freshwater flow, as discussed in other chapters of this report. Within the context of this chapter, these factors are the dispersion coefficient, which includes a tidal translation, and an advective coefficient, usually associated with the freshwater flow. It is also necessary to know the geometry and shape of the estuarine channel, since it affects these and other perameters.

With these data, the modeling effort proceeds as follows:

(1) Segmentation of the system. The estuary is divided into sections, the size of which depends on the computational scheme involved in the analysis of the water quality problem. In any case, the geometry, the hydraulic characteristics, tributaries, islands, inflow and tidal factors are the criteria which establish the bases for segmentation. Each segment has its own equation, either a finite-difference form of the differential equation or the general analytical solution of the differential, with its own set of coefficients. The segments are connected by flux concentration conditions which depend on the computational procedure.

(2) Coefficients of each segment. Each segment is charecterized by a set of geometric, hydrodynamic and reaction coefficients. The latter describe the various sources and sinks of dissolved oxygen. The former relate to the transport terms of dispersion and advection, which are usually evaluated by the longitudinal distribution of salinity.

(3) Oxidation coefficients. The reaction coefficients of biochemical oxidation may frequently be assigned by order of magnitude and checked by comparing the calculated profile with observations of the particular characteristics, i.e. carbonaceous BOD or TOC for the carbon, and

nitrogenous BOD or ammonia-nitrite for the nitrogen. In view of the usually low concentration of these substances and the inherent accuracy of the tests, such a comparison does not offer a method of exact refinement of these coefficients but indicates an approximate value, which may require further adjustment in view of the next step.

(4) Reaeration coefficient. This parameter may be evaluated by various formulae, which include the velocity and depth of the estuary. The temperature also is accounted for in the calculation of the reaeration coefficient.

(5) Comparison of computed profiles and observed data. With the information and coefficients available, the dissolved oxygen profile is computed and compared to observations. Because of the approximations and inaccuracies of both the parameters and data, it usually is not justified to employ a technique of best fit. A visual comparison is usually sufficient. If the comparison is favorable, the set of coefficients are tentatively accepted. If the computed profile does not agree with the observations, two factors are most frequently the cause: the sources of wastes and the oxidation coefficient. A thorough check on the various sources of waste water should be made and the approximation and estimates made in assigning magnitudes to these sources should be reviewed. Background values can sometimes be significant. If the BOD test is used, the ratio of the five-day to the ultimate value should be reanalyzed. If these are found to be satisfactory, the next coefficient to be adjusted is that of the oxidation process. Adjustment of these factors will usually account for discrepancies between calculations and observations. If more than one source of pollution exists, the principle of superposition applies; the effects of each are computed individually and added to determine the total.

(6) Evaluation at other conditions of model. Comparisons between observation and calculation should be made for various combinations of waste water discharge, temperature, freshwater flow and tidal conditions. The coefficients associated with the various processes may then be correlated to these parameters. Consistency in the relationships between the parameters of temperature, flow and tides on the one hand, and the coefficients of dispersion, advection, oxidation and reaeration, on the other, is the crux of the verification procedures. The greater the range of conditions evaluated and measured, the greater the certainty in interpolation and the greater the probability of realistic extrapolation. It is, of course, this process of either interpolation or extrapolation which provides the basis of the prediction procedure.

(7) Application of the model. Given the above, the model may be tentatively assumed to be verified, or at the very least adequate for purposes of prediction. Various engineering alternatives may now be quantitatively investigated and assessed, such as varying degrees and types of treatments, low-flow augmentation, flow diversions, and waste water relocations. In each case changes in the coefficients must be accounted for, particularly variations in the oxidation coefficient for various levels of waste treatment.

(8) Verification of model. The model may be considered verified if it has successfully predicted the change in water quality, after a significant change in the inputs to the system or a change in the estuarine environment itself has been made. Further modifications may be necessary and further data may have to be collected after changes are effected. It is this interplay between observations and modeling which yields the most fruitful approach to the development of water quality models.

2.6 MULTI-STAGE CONSECUTIVE REACTIONS (NITRIFICATION)

The BOD-DO case discussed in Section 2.4 is an example of a two-stage reaction. There are also several phenomena of importance in water quality management that are represented by a sequence of several forward reactions. These can be termed multi-stage consecutive reactions. If one is willing to accept a first-order kinetic assumption, bacterial nitrification can be thought of as a set of forward reactions which result in the conversion of various forms of nitrogen. The assumption of first-order kinetics is generally warranted if there are a large number of nitrifying bacteria present in the water. Nitrification is an important phenomenon in water quality management because of the significant amount of oxygen that may be utilized during the oxidation of ammonia nitrogen and nitrite nitrogen. In addition, several nitrogen forms may serve as a nutrient source for algal growth which upon death release nitrogen back into the system thereby completing the cycle. The incorporation of this feedback phenomenon is discussed in Section 7.1. In order to place the presentation of the multi-stage reaction in a specific problem context, nitrification of nitrogenous material will be used as the example, with no algal influences or feedback.

If N_1 , N_2 , N_3 and N_4 represent organic, ammonia, nitrite and nitrate nitrogen respectively, the bacterial nitrification phenomena can be represented as shown in Figure 3.4. Note that each of the nitrogen forms may also have direct waste inputs given by W_1 , W_2 , W_3 and W_4 . Each block incorporates the advection and dispersion in the estuary as described in the previous sections. If one is interested in describing the effect of nitrification on the DO resources of the estuary, the ammonia and nitrite outputs, as a first approximation, can be stoichiometrically converted to oxygen demands. The DO balance equation would therefore have two additional sink terms: the DO depletion due to the oxidation of NH_3 to NH_2 through the source of DO deficit given by $3.43\ K_{23}N_2$, and the depletion due to oxidation of NO_2 to NO_3 through the deficit source of $1.14\ K_{34}N_3$. Again, the sensitivity of these consecutive systems to the reaction coefficients is readily apparent in the form given in Figure 3.4.

The steady-state differential equations for this four-stage system are given in the context of nitrification by

$$0 = \frac{1}{A}\frac{d}{dx}\left(EA\frac{dN_1}{dx}\right) - \frac{1}{A}\frac{d}{dx}(QN_1) - K_{11}N_1 \qquad (3.26a)$$

$$0 = \frac{1}{A}\frac{d}{dx}\left(EA\frac{dN_2}{dx}\right) - \frac{1}{A}\frac{d}{dx}(QN_2) - K_{22}N_2 + K_{12}N_1 \qquad (3.26b)$$

$$0 = \frac{1}{A}\frac{d}{dx}\left(EA\frac{dN_3}{dx}\right) - \frac{1}{A}\frac{d}{dx}(QN_3) - K_{33}N_3 + K_{23}N_2 \qquad (3.26c)$$

$$0 = \frac{1}{A}\frac{d}{dx}\left(EA\frac{dN_4}{dx}\right) - \frac{1}{A}\frac{d}{dx}(QN_4) - K_{44}N_4 + K_{34}N_3 \qquad (3.26d)$$

The coefficients K_{ii} represent the first-order decay of substance i and combine oxidation effects and settling effects. The coefficients K_{ij} are the forward reaction coefficients and represent the source term of substance i feeding into substance j . Equations (3.26a)-(3.26d) therefore permit determination of the individual nitrogen components. As shown in Figure 3.4, the forcing functions for the DO deficit are $3.43\ K_{23}N_2$ and $1.14\ K_{34}N_3$, the first representing ammonia oxidation and the second nitrite oxidation. These inputs are then incorporated in the DO deficit equation and appropriate solutions obtained for each of the nitrogen forms.

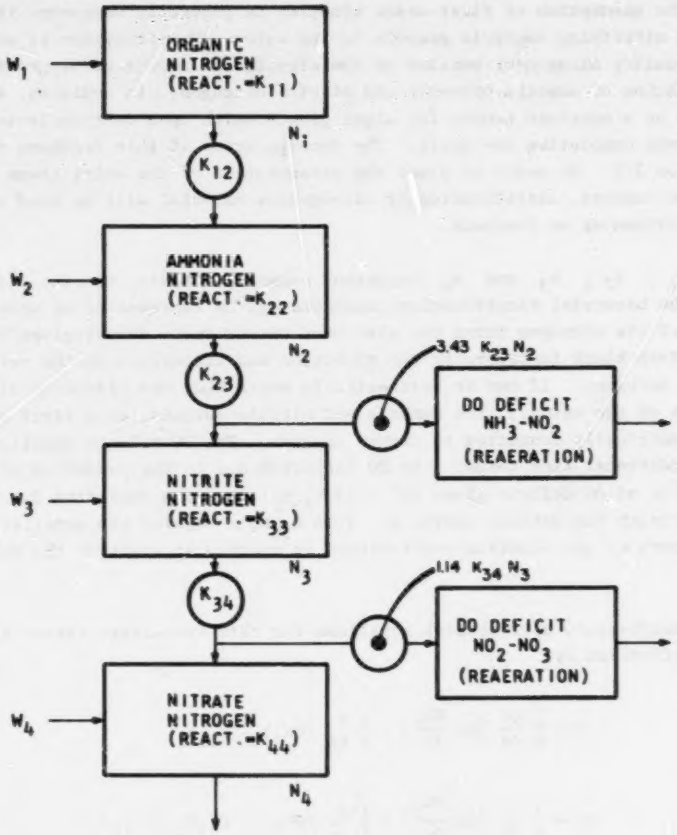

W1
ORGANIC NITROGEN (REACT.=K11)
N1
K12
W2
AMMONIA NITROGEN (REACT.=K22)
N2
K23
3.43 K23 N2
DO DEFICIT NH3-NO2 (REAERATION)
W3
NITRITE NITROGEN (REACT.=K33)
N3
K34
1.14 K34 N3
DO DEFICIT NO2-NO3 (REAERATION)
W4
NITRATE NITROGEN (REACT.=K44)
N4

Fig. 3.4 Consecutive reactions, nitrification phenomena.

An application of this feedforward multi-stage system was made for the Delaware Estuary (Thomann *et al*. 1970) assuming bacterial nitrification predominated in the system. For the Delaware, it is estimated that about 110,000 pounds/day of oxidizable nitrogen (organic and ammonia) is discharged from fifteen municipal and industrial sources (Hydroscience, Inc., 1969). The method of computation used was the continuous solution approach for the steady-state first-order kinetic case. Verification analyses were applied to a series of longitudinal profiles of the various nitrogen forms collected during different seasons. Results of one such verification run are shown in Figure 3.5. The ammonia profile was verified by utilizing a greatly reduced reaction rate in the reach from mile 100 to mile 85, a stretch of the estuary that coincides with low dissolved oxygen (less than 2 mg/l). The hypothesis is that the nitrification phenomenon is inhibited at these low concentrations. Verification of the relatively high levels of ammonia observed was not possible without this assumption. Other survey periods were also analyzed to provide a consistent set of reaction coefficients for each of the nitrogen forms. The nitrogen analyses then formed a basis for estimating the effects of nitrification on the dissolved oxygen deficit. The DO analysis indicated that with favorable conditions for nitrification, no nitrogen removal, and assuming that all oxidizable nitrogen was utilized in the bacterial nitrification stage, as much as 2.5 mg/l DO deficit could occur.

It should be noted that the classical BOD-DO equations described previously are a special case of these multi-stage reactions. For arbitrary coefficients, useful analytical solutions to Equations (3.26a)-(3.26d) are not available. For many purposes successive solutions can be obtained for constant coefficients. These solutions have forms similar to the BOD-DO solutions, Equation (3.23), and can be expressed in terms of a series of exponentials. This can readily be seen by recognizing that at any step in the consecutive reaction, the input from the preceding substance will be in terms of an exponential. For an exponential forcing function, the response of any equation of the form of Equations (3.26) is another exponential. The problem consists essentially of adequately accounting for boundary conditions and reaction coefficients. Alternatively, Equations (3.26) can be expressed in finite-difference form and the resulting set of algebraic equations can then be solved directly. Both solution techniques are discussed in Section 3.

2.7 DATA REQUIREMENTS

The previous discussions have generally indicated the relevant variables and parameters that must be examined in many estuarine water quality problems. It is appropriate to summarize here the data that are necessary for analyzing the effects of water quality control programs. There are obviously a wide variety of estuarine water pollution problems ranging from the relatively simple salt distribution problem to the more complex and highly interrelated algal dynamics problem. However, there are certain basic data requirements which can be stipulated and which will aid in placing relative weights on the modeling effort.

Data are most often lacking on the magnitude and characteristics of the waste water inputs. These inputs include direct discharges from municipal and industrial sources, storm water and combined sewage runoff and agricultural drainage. Determining the spatial and temporal variations of characteristics of these waste inputs is an expensive and time-consuming process. The only problem context in which this data requirement is not of paramount concern is when the loads do not yet exist and a simulation is being performed on the possible effect of some future load development. Many problem contexts, however, have required determination of both the present and future waste loads. Necessary sampling should include:

(a) Waste water physical characteristics

1. Flows, diurnal and seasonal variability, by-pass frequencies, combined overflows, land runoff
2. Temperature
3. Solids

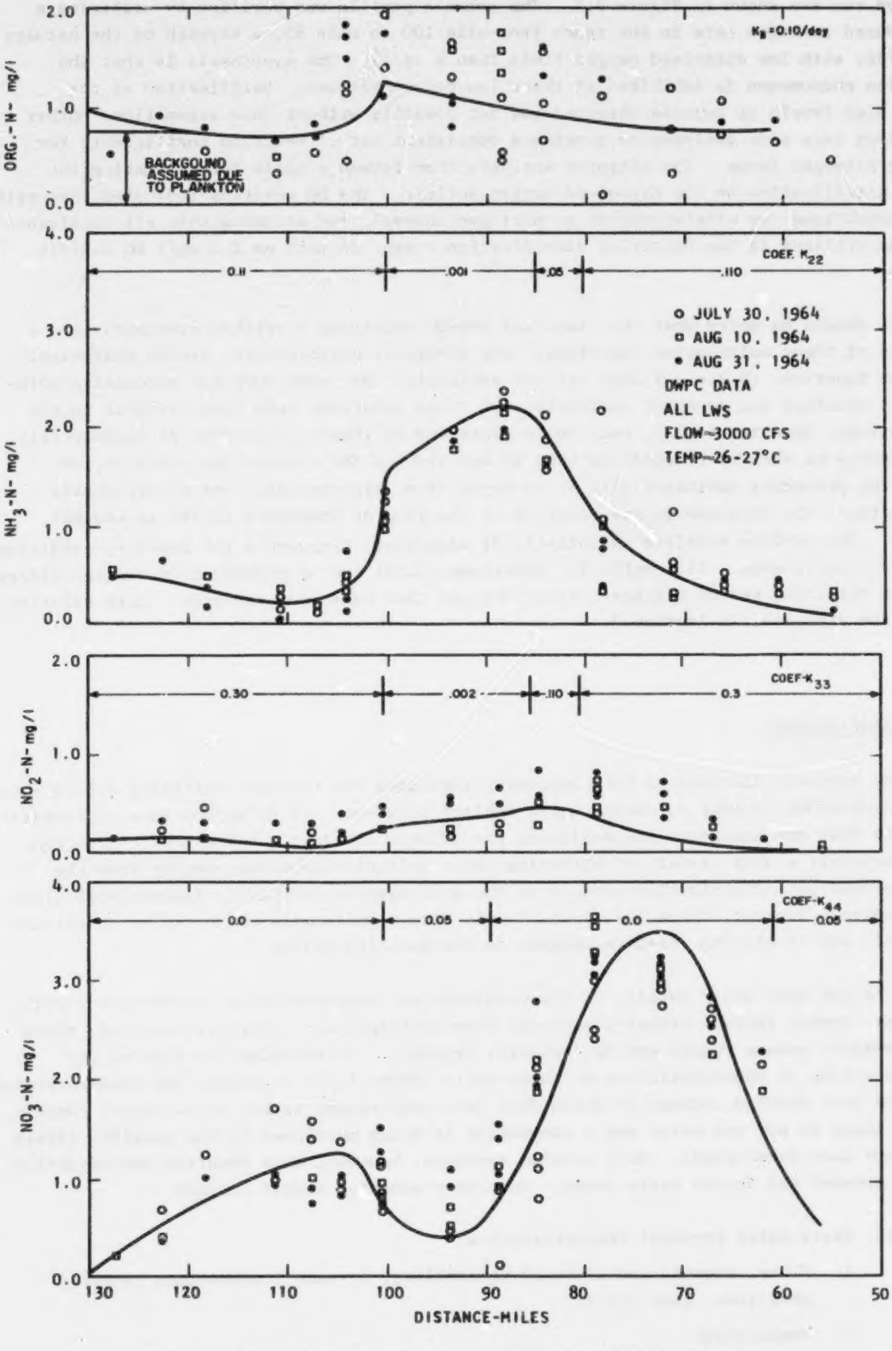


Fig. 3.5 **Comparison of observed and computed (solid line) organic, ammonia, nitrite and nitrate nitrogen - Delaware Estuary, August 1964.**

(b) Waste water quality characteristics

1. Carbonaceous BOD and nitrogeneous BOD (long-term BOD studies)
2. Nitrogen forms: organic, ammonia, nitrite, nitrate
3. Phosphorous forms: total, dissolved
4. Bacteria: total and fecal coliform, fecal streptococci
5. pH, acidity, alkalinity
6. Other variables that may be at potentially toxic levels

Not all analyses need be done on every waste source since problem contexts will differ. However, many estuarine water quality problem situations now demand a greatly expanded list of pertinent waste water characteristics to be determined. In terms of the number of samples, an attempt should be made to obtain data throughout a year on possibly a once-a-week daily-composite basis. Shorter term hour-to-hour waste water fluctuations may be important in some cases. As indicated previously, lack of definitive information on the waste load inputs may lead to poor approximations of load magnitude and variability with subsequent weakening of the model effort.

Data on the hydrologic and water quality characteristics of the estuary itself are also required and in some instances are more readily available than the waste water input data. In terms of sampling programs, data on the estuary itself are collected to provide some basis for the modeling effort including verification analyses. Generally such programs are relatively expensive and care must be taken that the problem context has been properly analyzed to insure that the proper time and space scales are being examined. Sampling generally includes:

(a) Estuarine hydrologic and physical characteristics

1. Meteorological variables, e.g. precipitation, wind
2. Solar radiation
3. Tidal range and velocities
4. Cross-sectional area
5. Water depth
6. Freshwater flow: time and space distribution
7. Salinity, chlorides
8. Temperature
9. Light extinction properties

(b) Estuarine water quality characteristics

1. Dissolved oxygen
2. BOD determination: oxygen uptake rate studies
3. Nitrogen forms
4. Phosphorous forms
5. Bacterial levels
6. pH, acidity, alkalinity
7. Other special variables related to specific waste discharges

(c) Estuarine biological characteristics

1. Total algal counts: species determinations and counts
2. Chlorophyll forms
3. Zooplankton
4. Vertebrates
5. Toxicity determinations

Again not all variables must be determined to the same degree for all problem contexts. However, many water quality estuarine situations require determinations of the water quality characteristics listed above together with the biological information, and it is precisely these characteristics that have demanded the greatest share of time and expense in estuarine sampling studies. Most of the physical paremeters are available or are readily obtained.

Occasionally, it may be desirable to carry out dye dispersion tests to determine the order of the intertidal dispersion coefficient. However, as pointed out previously one can obtain such estimates from salinity or other conservative tracers in the estuary. Alternatively, one can turn to numerical nonsteady-state models which do not require an estimate of the tidal dispersion coefficient (see Chapter II).

Estuarine water quality modeling, therefore, requires a complex sampling program which must obtain data on waste water inputs and receiving water quality. There are no rigorous rules for the time and space scales that must be examined; each problem context (including the available budget) determines the magnitude and sequencing of the number of samples that must be obtained and the analyses that must be performed.

3. SOLUTION TECHNIQUES FOR ONE-DIMENSIONAL STEADY STATE

3.1 AVAILABLE APPROACHES

Although the use of analytical solutions to the one-dimensional steady-state equation is helpful in gaining insight into the behavior of water quality in an estuary, for a number of practical problems complete analytical solutions are not always available. For certain functional forms of the system parameters analytical solutions may be obtained as indicated above, but as the size and complexity of the problem increases the equations become intractable and/or the solution becomes too cumbersome. Because of this difficulty, two approaches have been utilized to solve one-dimensional problems in estuaries.

The first approach, which can be called the continuous solution approach, makes use of the solutions to the constant-coefficient steady-state equation (see Equation 3.15). Most estuaries have hydraulic and geometric characteristics, such as cross-sectional area, depths, widths, and flows, which vary along the longitudinal axis of the channel from upstream to the ocean. In order to represent these variations mathematically, it is necessary to divide the system into a number of individual segments, each of which is characterized by its own physical and hydraulic parameters. The segments are then joined in a mathematical fashion, by means of boundary conditions relating concentration and flux of pollutant at each face of the junction. In this manner, changes in geometry, tributaries, dams, inflows, may all be incorporated into the mathematical definition of the system. Figure 3.6 illustrates the segmentation. Solutions are written down in terms of unknown coefficients which may be evaluated by means of a sequence of mass balance and concentration equalities. Continuous solutions are therefore obtained throughout each reach. A medium-size computer is usually required.

The second approach, which can be called the finite section approach, in essence replaces the derivatives in the steady-state equation with difference approximations. The estuary is divided into a number of sections (usually many more sections than in the continuous solution approach). It is assumed that each section is completely mixed so that continuous solutions are not obtained within each section. With each section the steady-state equation is therefore replaced by a series of algebraic equations, one equation for each finite section. Solution is obtained by matrix inversion or relaxation techniques. Depending on problem size, a medium to large computer is required.

The relative advantage of the continuous solution approach is that longer lengths of the estuary can be examined without resorting to a finite approximation. As such, the size of the matrix to be inverted is equal to or less than $2n$ where n is the number of reaches. In contrast, the finite section approach, because of the completely mixed approximation, requires more sections and the matrix to be solved becomes larger. As an example, where comparisons have been made, the continuous approach required solution of a 15 x 15 matrix while the finite section matrix was twice that size. In other situations, the disparity may be greater.

On the other hand, the logic surrounding the continuous solution approach tends to be complex and generalized systems are difficult to handle. The logic of the finite section approach is simple and for one-dimensional estuaries, the matrix is of a special form (tri-diagonal) allowing rapid computation. All possible analytical solutions must be programmed

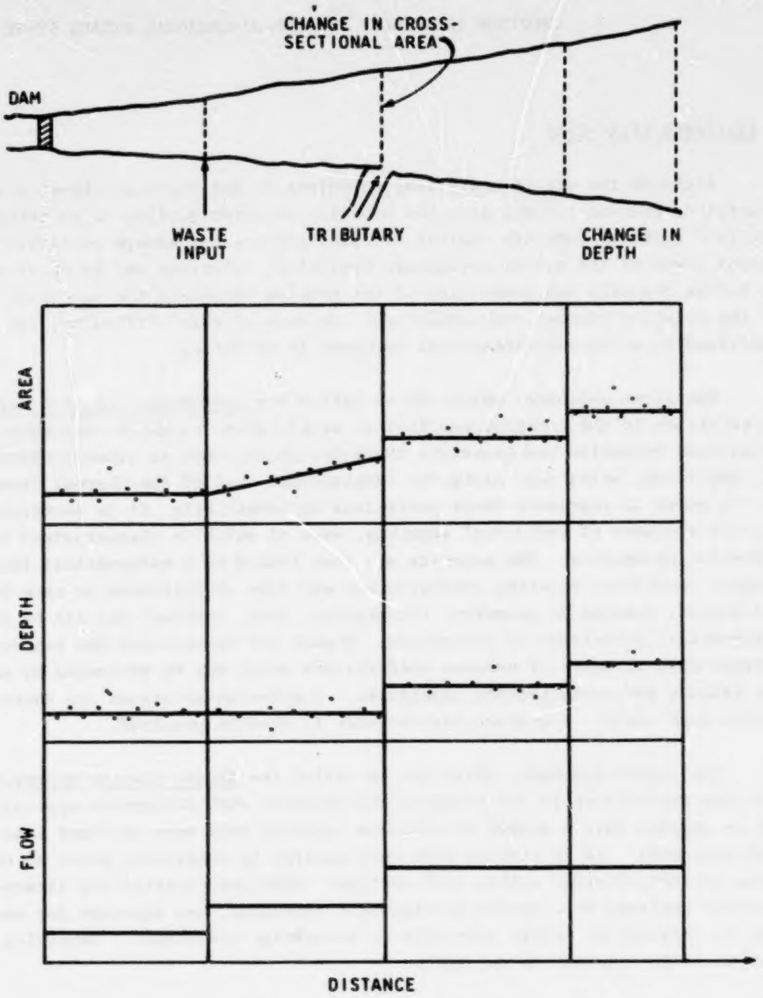

CHANGE IN CROSS-SECTIONAL AREA
DAM
WASTE INPUT
TRIBUTARY
CHANGE IN DEPTH
AREA
DEPTH
FLOW
DISTANCE

Fig. 3.6 Illustration of segmentation.

for the continuous solution approach including zero freshwater flow cases and uniform load cases. In the finite section approach, only one set of equations is programmed. The fundamental difference is that the continuous solution approach deals with solutions to the differential equation while the finite section approach deals with an approximation to the differential equation. Each will be considered here for some simplified cases.

3.2 CONTINUOUS SOLUTION APPROACH

A detailed review of the continuous solution approach is given elsewhere (Hydroscience, Inc., 1968 and O'Connor 1962). The general complementary solution to Equation (3.14) (constant parameters, steady state) is Equation (3.15), repeated here:

$$c = B \exp(gx) + C \exp(jx) \tag{3.27}$$

where B and C are unknown coefficients to be evaluated and g and j are given following Equation (3.16). If there is a uniformly distributed (in space) load entering the system, then the general solution is

$$c = B \exp(gx) + C \exp(jx) + \frac{W}{AK} \tag{3.28}$$

These equations form the building blocks from which complicated systems can be handled. A simple case will illustrate the use of these equations.

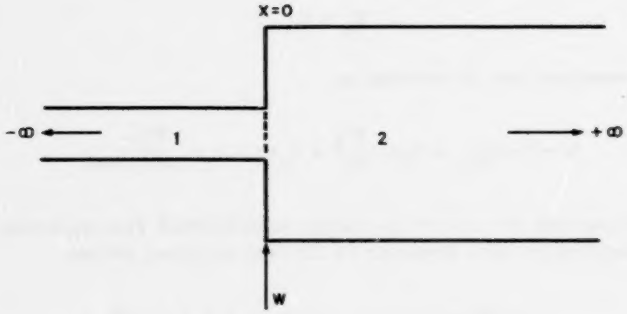


Fig. 3.7 A two-reach estuary.

Figure 3.7 shows an estuary with an incoming point waste load W at x = 0 . Upstream from this point, one or several of the system parameters (for example area and K) are different from the parameters downstream of the discharge point. The estuary is then divided into two reaches: reach 1 upstream and reach 2 downstream, as shown. All system parameters are then subscripted depending on reach location. Equation (3.28) is applied to each reach to give

$$\begin{aligned} c_2 &= B_1 \exp(g_1 x) + C_1 \exp(j_1 x) \\ c_2 &= B_2 \exp(g_2 x) + C_2 \exp(j_2 x) \end{aligned} \tag{3.29}$$

Note that g and j are also subscripted by reach. In order to obtain the complete solution to Equation (3.29), four boundary conditions are available:

a) $c_1 = 0$ at $x = -\infty$
b) $c_2 = 0$ at $x = +\infty$
c) $c_1 = c_2$ at $x = 0$
d) mass in = mass out at $x = 0$

The first boundary condition gives $C_1 = 0$ or

$$c_1 = B_1 \exp(g_1 x) \tag{3.30}$$

This is obtained by recalling that g is positive and j negative. Thus for $c_1 = 0$ at $x = -\infty$, $\exp(j_1 x)$ would be infinite unless $C_1 = 0$. The second boundary condition gives $B_2 = 0$ or

$$c_2 = C_2 \exp(j_2 x) \tag{3.31}$$

The third boundary condition yields at $x = 0$

$$B_1 = C_2 \tag{3.32}$$

The fourth boundary condition can be written as

$$W = \left[- Q_1 c_1 + E_1 A_1 \frac{dc_1}{dx} + Q_2 c_2 - E_2 A_2 \frac{dc_2}{dx} \right]_{x=0} \tag{3.33}$$

Evaluation of the derivatives at $x = 0$ is easily accomplished from Equation (3.30) and Equation (3.31). Substitution into Equation (3.33) and grouping yields

$$B_1(E_1 A_1 g_1 - Q_1) + C_2(Q_2 - E_2 A_2 j_2) = W \tag{3.34}$$

where Q_1 is the flow from the upstream reach to $x = 0$ and Q_2 is the flow out from $x = 0$ into the downstream reach. Positive Q is directed into the plane $x = 0$ and negative Q is directed outward from the plane $x = 0$. For many estuarine situations $Q_1 = Q_2$ which simplifies some of the elements.

Equations (3.32) and (3.34) can now be solved for the unknown coefficients B_1 and B_2 which together with Equations (3.30) and (3.31) provide the complete solution. In matrix form,

$$\begin{pmatrix} 1 & -1 \\ E_1 A_1 g_1 - Q_1 & Q_2 - E_2 A_2 j_2 \end{pmatrix} \begin{pmatrix} B_1 \\ C_2 \end{pmatrix} = \begin{pmatrix} 0 \\ W \end{pmatrix} \tag{3.35}$$

The complete solution is

$$c_1 = \frac{W}{E_1 A_1 g_1 - Q_1 - E_2 A_2 j_2 + Q_2} \exp(g_1 x) \tag{3.36}$$

and

$$c_2 = \frac{W}{E_1A_1g_1 - Q_1 - E_2A_2j_2 + Q_2} \exp(j_2x) \qquad (3.37)$$

For the special case of constant parameters everywhere: $E_1 = E_2 = E$; $A_1 = A_2 = A$; $Q_1 = Q_2 = Q$; and $K_1 = K_2 = K$. Equations (3.36) and (3.37) reduce to Equations (3.16) and (3.17). This example illustrates the use of the continuous solution approach for the simple case of two reaches with differing parameters extending upstream and downstream from a point waste source.

If at some distance downstream, a new reach is necessary because of a change in one of the system parameters or because of a new waste load, a similar procedure is followed. In this case, new unknown coefficients are introduced and the matrix becomes larger. There will now be three equations, one for each reach as

$$\begin{aligned} c_1 &= B_1 \exp(g_1x) + C_1 \exp(j_1x) \\ c_2 &= B_2 \exp(g_2x) + C_2 \exp(j_2x) \qquad (3.38) \\ c_3 &= B_3 \exp(g_3x) + C_3 \exp(j_3x) \end{aligned}$$

Concentration equalities are now formed and, together with the mass balance equations, will provide four equations in four unknown coefficients. Although there are six unknown coefficients in Equation (3.38), C_1 and B_3 are zero because of the minus infinity and plus infinity boundary conditions. The situation is now more complex because one of the coefficients, either B_2 or C_2, for the middle reach cannot be eliminated. The distance from $x = 0$ (point of discharge) to the beginning of the next downstream reach is designated x_o. It can be shown that four equations in four unknowns (B_1, B_2, C_2 and C_3) result from the application of the boundary condition. Simultaneous solution provides the values of the unknown coefficients for use in Equations (3.38) (Thomann 1970).

This approach is a powerful technique for dealing with one-dimensional estuarine systems. The system can be made as complex as desired. The logic of constructing the elements of the matrix must be carefully followed and appropriate boundary conditions must be used. Infinity conditions are not always possible (as in the case of dams) in which case special boundary conditions can be utilized.

3.3 FINITE SECTION APPROACH

This approach (Thomann 1963), instead of employing various solutions to the steady-state equation (3.14), considers the differential equation directly. Continuous space is replaced by finite volumes that are assumed to be completely mixed. Material balances are then written around each finite length of estuary. The finite section approach is essentially a finite-difference approximation to an ordinary differential equation.

Figure 3.8 shows the length of the estuary divided into N sections. The first section is usually placed at the head end of the estuary or sufficiently far upstream from the last major waste outfall. There are two similar derivations that may be used to determine the

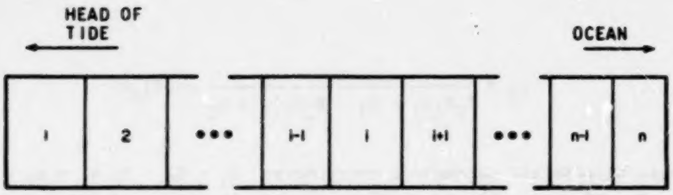


Fig. 3.8 Finite section segmentation for one-dimensional estuary.

necessary computation formulas. Both derivations give the same result. The first derivation constructs a model on physical reasoning by writing a mass balance equation around a finite volume similar to the technique used in constructing Equation (3.14). The second derivation starts with Equation (3.14) and approximates each of the derivatives.

Using the first derivation, one proceeds by writing a mass balance around section i of the estuary. Each section is considered to be a mixed volume. No gradients are permitted in the sections. The time rate of change of material c_i in section i is then given by

$$V_i \frac{dc_i}{dt} = Q_{i-1,i}\left[\alpha_{i-1,i}c_{i-1} + \beta_{i-1,i}c_i\right] - Q_{i,i+1}\left[\alpha_{i,i+1}c_i + \beta_{i,i+1}c_{i+1}\right] \tag{3.39}$$

$$+ E'_{i-1,i}(c_{i-1}-c_i) + E'_{i,i+1}(c_{i+1}-c_i) - K_iV_ic_i + W_i \pm \Sigma_i;\ i = 1,2\ldots N$$

where

V_i = volume of segment i

E'_{ij} = bulk dispersion coefficient = $E_{ij}A_{ij}/\bar{L}$ where $\bar{L}$ is the average length of adjacent sections

α_{ij} = dimensionless mixing coefficient; $\beta = 1 - \alpha$

Σ_i = sources and sinks of c

The parameter α_{ij} is, in mathematical terms, a finite-difference weight. For $\alpha = 1/2$, a central difference approximation of the derivative is utilized while for $\alpha = 1$, a backward difference approximation is used. In physical terms, α can be related to the ratio of the dispersion to advective forces and it can be shown that $\alpha > 1 - E'/Q$ (Thomann 1970). If all terms in c_{i-1}, c_i and c_{i+1} are grouped on the left side, one obtains

$$a_{i,i-1}c_{i-1} + a_{ii}c_i + a_{i,i+1}c_{i+1} = W_i$$

as the general equation for the i^{th} section where a_{ij} are functions of V, Q, E′, α and K. For the upper and lower boundary sections, a similar derivation indicates that the incoming and exit boundary concentration can be incorporated into W_1 and W_n. The n equations can be written in matrix form as

$$[A](c) = (W) \tag{3.40}$$

where [A] is an n x n matrix and (c) and (W) are n x 1 vectors. The solution vector (c) is then obtained by multiplying through by the inverse of the A matrix or

$$(c) = [A]^{-1}(W) \tag{3.41}$$

The problem then of determining the steady-state one-dimensional distribution of waste material in an estuary with spatially variable parameters reduces to solving n simultaneous algebraic equations (Equation 3.40) or inverting an n x n matrix (Equation 3.41).

The matrix [A] has a particular form for the one-dimensional estuary. This form is known as a tri-diagonal matrix where only the main diagonal and the diagonals above and below the main diagonal appear in the matrix. All other elements are zero. This is a feature which permits special efficient computing programs for determination of the inverse $[A]^{-1}$. One can of course use other methods of solution of simultaneous equations (e.g. Gauss-Seidel technique) to obtain the concentrations in each section.

The inverse matrix $[A]^{-1}$ is termed a steady-state response matrix and represents the responses in c due to the discharge of material of a unit amount into each section. This can be seen by

$$[A][c] = [I]$$

or (3.42)

$$[c] = [A]^{-1}[I]$$

where [I] is the identity matrix and [c] is now an n x n matrix. The first column of [c] then represents the response over all sections due to a unit steady input into the first section, the second column of c represents the response over all sections due to a unit steady input into the second section, and so on.

For two-stage consecutive reactions, as in the case of carbonaceous BOD-DO, a similar procedure is followed. A matrix [B] is generated; the only difference between [A] and [B] is the reaction coefficients on the main diagonal. Thus let D stand for DO deficit and L for BOD. The matrix equation for DO is

$$[B](D) = (\Sigma)$$

where (Σ) is the vector of sources and sinks. If only the BOD sink of DO is considered then

$$[B](D) = (VK_dL)$$

where K_d is the deoxygenation coefficient. Multiplying by $[B]^{-1}$ gives

$$(D) = [B]^{-1}(VK_dL)$$

But since

$$\left(L\right) = \left[A\right]^{-1}\left(W\right)$$

then

$$\left(D\right) = \left[B\right]^{-1}\left[VK_d\right]\left[A\right]^{-1}\left(W\right) \tag{3.43}$$

where $[VK_d]$ is an n x n diagonal matrix. Equation (3.43) indicates the method of solution for two stage consecutive reactions. (See also Bunce and Hetling 1966 and Hetling and O'Connell 1966 for other discussions and applications of this approach.)

The solution technique in terms of the finite section approach for multi-stage consecutive reactions is now clear. Thus, consider the case of the four nitrogen forms designated as N_1 = organic nitrogen , N_2 = ammonia nitrogen , N_3 = nitrite nitrogen and N_4 = nitrate nitrogen . The matrix equations are

$$\begin{aligned}
\left[A_1\right]\left(N_1\right) &= \left(W_1\right)\\
\left[A_2\right]\left(N_2\right) &= \left(W_2\right) + \left(VK_{12}N_1\right)\\
\left[A_3\right]\left(N_3\right) &= \left(W_3\right) + \left(VK_{23}N_2\right)\\
\left[A_4\right]\left(N_4\right) &= \left(W_4\right) + \left(VK_{34}N_3\right)
\end{aligned} \tag{3.44}$$

where K_{ij} are the "forward" reaction coefficients and the $[A_i]$ differ only on the main diagonal by the differences in the reaction coefficients K_{ii} . The solution for (N_3) is given as an example. Substitution of successive solutions of (N_1) and (N_2) into the equation for (N_3) gives the solution as

$$\begin{aligned}
\left(N_3\right) = &\left[A_3\right]^{-1}\left(W_3\right) + \left[A_3\right]^{-1}\left(VK_{23}\right)\left[A_2\right]^{-1}\left(W_2\right)\\
&+ \left[A_3\right]^{-1}\left(VK_{23}\right)\left[A_2\right]^{-1}\left(VK_{12}\right)\left[A_1\right]^{-1}\left(W_1\right)
\end{aligned} \tag{3.45}$$

Again, the solution vector need not be obtained by matrix inversion, but rather more efficient routines for solution of simultaneous equations can be used.

This methodology can be applied to the multi-stage consecutive reactions described above and forms the basis for the feedback model described in Section 7.1.

4. TWO-DIMENSIONAL STEADY STATE

The steady-state mass balance equation for single-stage non-conservative substances in two dimensions is given by

$$\frac{\partial c}{\partial t} = 0 = -\frac{\partial}{\partial x}(uc) - \frac{\partial}{\partial y}(vc) + \left(\frac{\partial}{\partial x}\left(E_x \frac{\partial c}{\partial x}\right)\right) + \left(\frac{\partial}{\partial y}\left(E_y \frac{\partial c}{\partial y}\right)\right) - K(x,y)c \tag{3.46}$$

where u and v are the velocities in the x- and y- direction and similarly E_x and E_y are the tidal dispersion coefficients in the x- and y- direction. These two directions can be interpreted in terms of either the horizontal plane (x - length, y - width) or the vertical plane (x - length, y - depth). General analytical solutions of Equation (3.46) for arbitrary coefficients are not available. Hence, in water quality modeling, various assumptions are usually made in the system parameters or for variable parameters a finite section approach can be used. Forms of Equation (3.46) have been applied to the vertical distribution of salt in salt water wedge estuaries and fjords (Hansen 1967, Rattray and Hansen 1962). Other applications in water quality studies of wide estuaries or bays have generally been limited. A finite section approach was used in studying the lateral distribution of salinity in Raritan Bay and Hillsborough Bay (Hagan and Gallagher 1969). Other work is being done on the application of a finite-difference form of Equation (3.46) to two-dimensional distribution of such water quality variables as bacteria, BOD and DO in Boston (Hydroscience 1970) and San Juan Harbors. A pseudo-two-dimensional approach has also been used in the San Francisco Bay area (Orlob et al. 1967) and the Columbia estuary (Callaway et al. 1969). In these cases, the two-dimensional aspects are introduced by coupling one-dimensional channel sections. This requires an a priori specification of the directions in which gradients will occur. A complete two-dimensional nonsteady-state analysis has been used in Jamaica Bay in New York City (Leendertse 1970). This work requires solution of the two-dimensional equations of motion together with water quality modeling. It probably represents one of the more advanced truly two-dimensional analyses to date. As increased attention is turned to the bay and harbor case, one can expect further application of two-dimensional models.

4.1 SOLUTION APPROACH: FINITE DIFFERENCE

One approach to solving Equation (3.46) is to utilize the notion of a sequence of completely mixed sections discussed in terms of the one-dimensional estuary in Section 3. For the multi-dimensional steady-state case, a mass balance around a finite section k surrounded by segments j is given (Thomann 1963) as (see Figure 3.9)

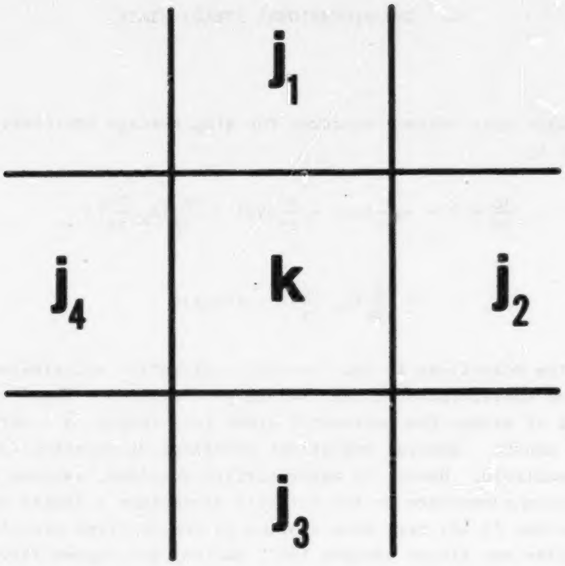


Fig. 3.9 Segmentation in two dimensions.

$$V_k \frac{dc_k}{dt} = 0 = \sum_j \left[-Q_{kj}(\alpha_{kj}c_k + \beta_{kj}c_j) + E'_{kj}(c_j - c_k) \right]$$

$$- V_k K_k c_k + W_k \pm \Sigma_k ; \; k = 1,2 \ldots n \tag{3.47}$$

where all terms have been defined previously and the summation extends over all j segments bordering on segment k . This equation also results from a formal finite-difference approximation to Equation (3.46) with a variable weight given to the advective term. If all terms involving the dependent variable c_k are grouped on the left hand side, one obtains

$$a_{kk}c_k + \sum_j a_{kj}c_j = W_k \pm \Sigma_k \tag{3.48}$$

where

$$a_{kk} = \sum_j (Q_{kj}\alpha_{kj} + E'_{kj}) + V_k K_k$$

$$a_{kj} = Q_{kj}\beta_{kj} - E'_{kj}$$

The flow convention is positive leaving the section. Note that

$$Q_{jk}\alpha_{jk} = Q_{kj}\beta_{kj}$$

and

$$Q_{jk}\beta_{jk} = Q_{kj}\alpha_{kj}$$

For sections on a boundary where the flow between the boundary and the section is designated Q_{kk} (positive leaving the section),

$$a_{kk} = \sum_j (Q_{kj}\alpha_{kj} + E'_{kj}) + V_k K_k + Q_{kk}\alpha_{kk} + E'_{kk}$$

and the forcing function is

$$W_k = W_k + (E'_{kk} - Q_{kk}\beta_{kk})c_B$$

where c_B is the boundary concentration. For Q_{kk} entering the section from the boundary (negative),

$$a_{kk} = \sum_j (Q_{kj}\alpha_{kj} + E'_{kj}) + V_k K_k + Q_{kk}\beta_{kk} + E'_{kk}$$

and

$$W_k = W_k + (E'_{kk} - Q_{kk}\alpha_{kk})c_B$$

The n equations with suitable incorporation of boundary conditions can be represented in matrix form as

$$\begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & & a_{2n} \\ \cdot & & & \cdot \\ \cdot & & & \cdot \\ \cdot & & & \cdot \\ a_{n1} & a_{n2} & & a_{nn} \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ \cdot \\ \cdot \\ \cdot \\ c_n \end{pmatrix} = \begin{pmatrix} W_1 \\ W_2 \\ \cdot \\ \cdot \\ \cdot \\ W_n \end{pmatrix} \qquad (3.49)$$

or

$$[A](c) = (W)$$

where $[A]$ is an $n \times n$ matrix of known coefficients that depends on the system parameters. For most applications, a relatively large number of the elements of $[A]$ are zero. The multi-dimensional matrix can be compared to the tri-diagonal form for one-dimensional estuaries.

It is important to note that the use of this approach requires an a priori specification of the net flow vectors and tidal dispersion fields. For some cases, it may be possible to route the freshwater flow component without resorting to complex hydrodynamic analyses.

In general, however, it will usually be necessary to model the two-dimensional hydrodynamic equations (see Chapters II and VI) to obtain an estimate of the distribution of the net advective flow. This requires integration of the hour-to-hour tidal velocities to determine the net flow patterns. For steady-state analyses, if one has estimates of the distribution of net advective flows (Q_{jk}) then the salinity or chloride two-dimensional surface can be used to obtain estimates of the intertidal dispersion coefficients. Alternatively one can run a time-variable two-dimensional model with the hydrodynamic equations and water quality mass conservation equation (Leendertse 1970) on an hour-to-hour prototype time scale thereby eliminating, for most purposes, concern with the tidal dispersion coefficient (E'_{kj}). Two difficulties arise: (1) computation time is increased greatly at those small time scales, and (2) the transition from that time scale to scales of seasons and years is not clear.

In any case, the steady-state multi-dimensional water quality problem (note that in principle a third dimension is included in the above development) reduces to solving n simultaneous equations or inverting matrix $[A]$ in Equation (3.49) provided an estimate of the net flow and dispersion fields is available. There are several advantages to obtaining the inverse matrix of $[A]$. Each column of the inverse indicates the water quality response in all sections due to a unit load in a specific location. This often proves useful for rapid assessment of load location or magnitude changes. During verification analyses, however, relaxation techniques for solving simultaneous equations are much more efficient. It can be shown that for a solution vector (c) that is positive everywhere, all elements off the main diagonal of $[A]$ should be negative. This provides a bound on the advection coefficient α which relates to the dispersion and advection forces (see discussion of Equation 3.39). Various algorithms are readily available for solving large systems of equations. For example, operational programs have been written for the IBM 1130 using disc storage to handle multi-dimensional water quality problems of up to 120 sections. Larger machines permit even greater numbers of sections up to at least 500 sections and with special programming techniques up to about 1,000 sections if necessary.

5. ONE-DIMENSIONAL TIME-VARIABLE MODELS

The equations for the one-dimensional time-variable water quality model for two-stage reactions, such as BOD and DO, are given by

$$\frac{\partial L}{\partial t} = -\frac{1}{A}\frac{\partial}{\partial x}(QL) + \frac{1}{A}\frac{\partial}{\partial x}\left(EA\frac{\partial L}{\partial x}\right) - K_r L \qquad (3.50)$$

$$\frac{\partial c}{\partial t} = -\frac{1}{A}\frac{\partial}{\partial x}(Qc) + \frac{1}{A}\frac{\partial}{\partial x}\left(EA\frac{\partial c}{\partial x}\right) + K_a(c_s - c) - K_d L + P - R - B \qquad (3.51)$$

Equation (3.50) can obviously be used to describe a single conservative variable such as chlorides where $K_r = 0$.

A temporal variation of the following parameters or inputs is usually present: freshwater flow, temperature, waste water discharge, and certain biological, chemical, and physical reactions. Furthermore, there are various time scales over which these variations may be significant. For a particular situation, a prescribed period of time is established for the analysis, and a unit of time is assigned. For example, if it is desired to study the quality variations of a natural body over the period of a year, it is probable the unit of time would be a day, perhaps a week or a month. If on the other hand, the period of concern is a day, obviously the time unit would be in the order of minutes or perhaps hours. The purpose of the analysis, the nature of the phenomena, and the order of the temporal variations contribute to the assignment of the scale and unit of time. Finally the variations observed can be thought of as varying in a statistically and random fashion or in a deterministic and prescribed manner. Thus, natural phenomena such as the temperature variations of the year and the sunlight over the day may be approximated by a cyclic function on which is superimposed a random variation. The discernible periodic fluctuations are usually evident. However, over smaller or larger time scales, the random nature of some phenomena may be more significant and without any apparent periodic form. One of the first steps in the analysis, therefore, is the assignment of the time scale of interest and unit of analysis, from which the choice of various functional forms of the temporal variations follow and the approximate methods of solution employed in the calculation. Equations (3.50) and (3.51) as they stand are quite general in their time scale of application. Intratidal time scales have been used to describe short-term and locally important quality gradients. Intertidal time scales extending out to seasonal variations have also been used to describe longer term fluctuations and larger scale spatial gradients.

Analyses of water quality in natural waters discussed previously in this chapter have concentrated on steady-state solutions. One of the critical questions which arises in this regard is the time interval required to establish the steady state. This period varies depending on the nature of the system, which includes the reaction, dispersion and advection coefficients. Thus from the hydrological point of view, in a freshwater stream the steady state may be quickly established and just as readily disrupted, while in the estuary a longer period is required because of the presence of dispersion. In the former case, the interval may be hours or days, while in the latter weeks or months.

5.1 SOLUTION APPROACH

Several approaches are presently available for dealing with the time-variable estuarine water quality model depending on the time and space scale of application (see Orlob et al. 1967, Leendertse 1970, Jeglic 1966, Pence et al. 1968). For many problem contexts, the minimum time interval is on the order of tidal cycles, although for other problem contexts shorter time scales are necessary. One method of solving the time-variable model with arbitrary inputs and coefficients is to replace the partial differential equations with a finite-difference scheme. Continuous space is then replaced by discrete finite spatial elements which are assumed to be homogeneous. Thus the finite section approach discussed previously is used, with the exception that the time derivative is not set to zero. For the BOD and DO systems, this results in a sequence of linear ordinary differential equations with time as the independent variable. One equation for each finite reach represents the waste-load-to-estuarine-BOD transformation, and the second equation for each reach represents the BOD-to-DO transformation. For n reaches, then, there are $2n$ differential equations to be solved.

This time-variable problem, requires that a numerical integration scheme be used. A variety of numerical schemes are available, and care must be taken that a scheme is adapted that is appropriate for the problem context. Short-term models have been used in Jamaica Bay (Leendertse 1970) and San Francisco Bay Studies (Orlob et al. 1967). Longer term models have been used in the Delaware (Jeglic 1966) and Potomac estuaries (Bunce and Hetling 1966, Hetling 1968). An extended discussion of differencing schemes is given in Chapter VI. A brief review is given here of the approach used in the Delaware and Potomac work.

Equation (3.50) will be used as an illustration of a differencing scheme that can be used in time-variable problems. The region of interest along the length of the estuary is segmented into n finite volume segments. The region of $L(x,t)$ in the vicinity of the k th segment will be examined and an approximation to Equation (3.50) in this region can be developed. Figure 3.10 shows the notation, where V is the volume of the segment and x the length of the segment.

One finite-difference approximation to the first derivative is given by

$$\left(\frac{\partial L}{\partial x}\right)_k \approx \frac{L_{k,k+1} - L_{k-1,k}}{\Delta x} \tag{3.52}$$

The second derivative approximation is given by the derivative of (3.52) evaluated at $x = k$ or

$$\left(\frac{\partial^2 L}{\partial x^2}\right)_k \approx \frac{1}{\Delta x}\left[\left(\frac{\partial L}{\partial x}\right)_{k,k+1} - \left(\frac{\partial L}{\partial x}\right)_{k-1,k}\right] \approx \frac{1}{\Delta x^2}\left[L_{k+1} - 2L_k + L_{k-1}\right]$$

The advective term on the right side of Equation (3.50) can then be written as

$$-\frac{1}{A}\frac{\partial}{\partial x}(QL) \approx -\frac{1}{A_k \Delta x}\left[(QL)_{k,k+1} - (QL)_{k-1,k}\right]$$

Similarly, the difference approximation for the second term, the dispersion term, gives

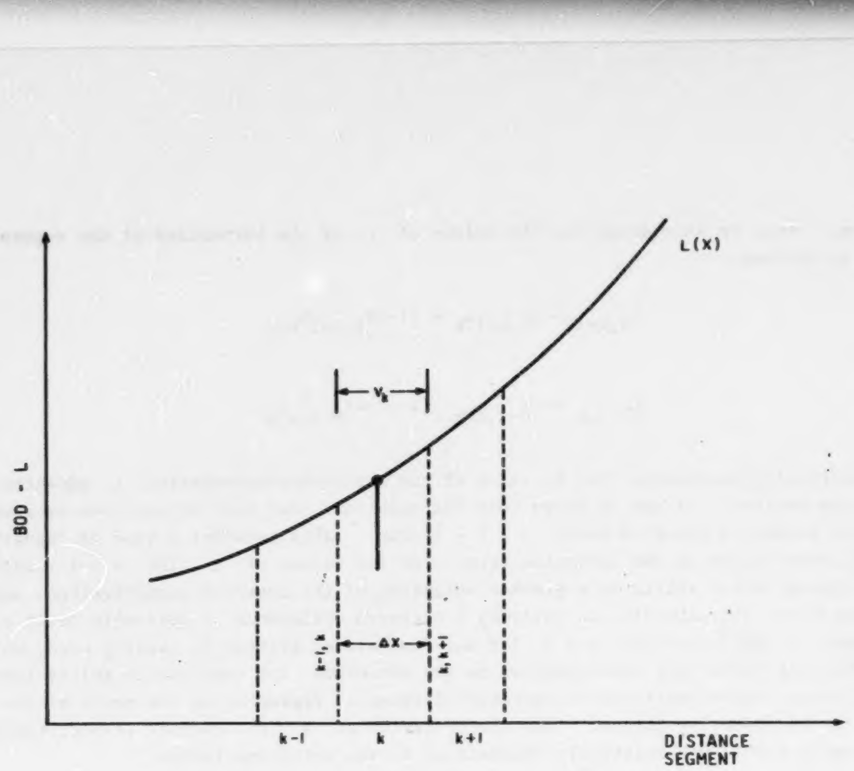


Fig. 3.10 Segmentation of longitudinal direction.

$$\frac{1}{A}\frac{\partial}{\partial x}(EA\frac{\partial L}{\partial x}) \approx \frac{1}{A_k \Delta x^2}\left[E_{k,k+1}A_{k,k+1}(L_{k+1}-L_k) - E_{k-1,k}A_{k-1,k}(L_k-L_{k-1})\right]$$

Equation (3.50) can then be rewritten in terms of finite spatial coordinates, and hence as an ordinary differential equation in time, as follows:

$$\begin{aligned} V_k \frac{dL_k}{dt} &= -\left[(QL)_{k,k+1} - (QL)_{k-1,k}\right] \\ &+ \frac{1}{\Delta x}\left[(EA)_{k,k+1}(L_{k+1}-L_k) + (EA)_{k-1,k}(L_{k-1}-L_k)\right] \qquad (3.53) \\ &- V_k K_k L_k + W_k \end{aligned}$$

where $V_k = A_k L$.

Equation (3.53) represents an approximation to the continuous form of Equation (3.50) and can be used for those cases involving arbitrary coefficients. One must guarantee physically realizable results in terms of solutions that are positive everywhere. One method of accomplishing this is to introduce a variable finite-difference weight for the advective term in the equation. Thus, an expression for the values of L at the boundaries of the segments can be written as follows:

$$L_{k,k+1} = \alpha_{k,k+1}L_k + (1-\alpha)_{k,k+1}L_{k+1}$$

and

$$L_{k-1,k} = \alpha_{k-1,k}L_{k-1} + (1-\alpha)_{k-1,k}L_k \tag{3.54}$$

where α physically represents that fraction of the upstream concentration L advected into the downstream section. It can be shown that for solutions that must be positive everywhere (the physical condition required here) $\alpha > 1 - EA/Q\Delta x$. This provides a type of changing difference approximation to the advective term. For low values of E , the $\alpha > 1 - EA/Q\Delta x$ difference approximation shifts to a greater weighting of the upstream concentration, and at zero dispersion the approximation is entirely a backward difference, a desirable trait of the approximation. A lower bound of $\alpha = \frac{1}{2}$ for one-dimensional systems is usually used, which indicates that the difference approximation to the advective term continually shifts from a central-difference approximation to a backward difference, depending on the ratio of the dispersion to the advective forces. Once the criterion of $\alpha > 1 - EA/Q\Delta x$ is met, the solutions are highly stable and relatively insensitive to the weighting factor.

Substituting Equation (3.54) into (3.53) gives

$$V_k \frac{dL_k}{dt} = Q_{k-1,k}\left(\alpha_{k-1,k}L_{k-1}+\beta_{k-1,k}L_k\right) - Q_{k,k+1}\left(\alpha_{k,k+1}L_k+\beta_{k,k+1}L_{k+1}\right)$$
$$+ E'_{k-1,k}\left(L_{k-1}-L_k\right) + E'_{k,k+1}\left(L_{k+1}-L_k\right) - V_kK_kL_k + W_k \tag{3.55}$$

where $Q_{ij} = A_{ij}u_{ij}$, and $E'_{ij} = E_{ij}A_{ij}/\Delta x$ and $\beta = 1 - \alpha$. Equation (3.55) expresses the time rate of change of L_k in terms of the concentration in the downstream segment L_{k+1} . This equation also results when a simple material balance is taken around each segment (see also Section 3.3). The first term then represents the amount of L advected into the segment. the second term represents the amount of L advected out of the segment, the third and fourth terms represent the dispersion effect, proportional to the concentration difference between the two segments, and the fifth term represents the decay of L in segment k .
It should be noted that in Equation (3.55), the time scale is arbitrary and the numerical schemes that have been developed (Orlob et al. 1967, Leendertse 1970, Jeglic 1966) can be applied equally to within-tidal analyses or longer time scales. The choice is left to the analyst after careful examination of the problem context.

It should be recognized that the use of finite section approximations introduces a numerical or psuedo-dispersion effect into the model. This can readily be seen when it is realized that each segment is assumed to be completely mixed. An impulse input is therefore immediately mixed in the volume not because of any physical effects but solely because of the numerical procedure. The amount of dispersion so introduced is given by $u\Delta x/2$ which provides an estimate for determining the relative amount of numerical dispersion compared to "true" dispersion. A detailed analysis of this effect is given in Bella and Dobbins (1968). For short time scale applications in estuaries, this numerical dispersion may be severe and lead to distorted results. For "low frequency" studies in turbulent estuaries where time scales of days to seasons are important as opposed to hours, this effect is not as significant.

In a simplified form, the equations to be solved can be written as

$$\frac{dL_k}{dt} = f(t, L_{k-1}, L_k, L_{k+1}) \tag{3.56}$$

and

$$\frac{dc_k}{dt} = g(t, c_{k-1}, c_k, c_{k+1}) \tag{3.57}$$

Basically, the computational procedure used in Jeglic (1966) begins from a set of initial values at time zero and in all segments, $k = 1 \ldots n$. Numerical integration is utilized to pull the solution one time step forward. After each step is completed, the new values of L_k and c_k are downgraded to become the initial values of the next step. The process is continued until the entire time span that is originally specified has been completed. Jeglic (1966) controls truncation errors by a halving and doubling procedure which, while sacrificing some computional time, does not require the user to specify an integration interval.

The computer program used in the Delaware case (Pence et al. 1968) for solution of the general time-variable estuary program is relatively large and designed primarily for machines of the size of an IBM-360, Model 65, or CDC 6600. In the application of the program to the Delaware Estuary the river was divided into thirty reaches. Primary emphasis was placed on the longer time scales (seasonal effects) so that the equations were used with a day as the basic prototype time unit. The dispersion coefficients used represented the tidal mixing effects, from one tide stage to the next. The integration interval was between four steps and fifteen steps per prototype day. The average problem for the Delaware required about four computer minutes per simulated month on an IBM-7094. This included seasonal variations in temperature and freshwater flow. Jeglic (1966) has given a rough gauge for overall running time as

Each integration time (milliseconds) = 20 · number of estuary sections

Shubinski et al. (1965) and Orlob et al. (1967) have used a similar approach to the one-dimensional diffusion-advection equation in applications to water quality problems in the San Francisco Bay area. In that work, primary attention is given to the shorter term, within-tidal cycle oscillations. As such, the tidal mixing phenomenon, which is incorporated above in the dispersion term, is of lesser consideration and primary interest centers about the advection term. Several forms of difference approximations were considered so that numerical mixing and stability factors were balanced. A "quarter-point" approximation to the advective term was finally used. This is in contrast to the time-dependent model used in the Delaware where a variable difference approximation to the advective term is used. In that case, guarantee of positive solutions is maintained by continually checking the ratio of dispersion to advection.

6. VERIFICATION

In the discussion above, the assumption was made that the system parameters and inputs are known. However, it is usually difficult to specify the values of the system parameters *a priori*. Although the order of magnitude of all of the parameters and usually most of the inputs is known, from either empirical correlations or fundamental analyses, the means for more precise independent specification for many of the terms in the equations are not presently available. Consequently, for coupled systems such as the DO problem, Equations (3.16) and (3.23) in conjunction with field data may be used to evaluate one or all of the coefficients. The nontidal advective component U is most readily determined by the hydraulic continuity relation, regardless of the small difficulty involved in obtaining representative values of the flow and area. Conservative tracers, such as salt from the ocean or a stable chemical from a waste source, may be used in Equation (3.13) to determine the tidal dispersion coefficient, if the advection due to freshwater inflow is known. With these two coefficients, the first reaction coefficient may be obtained from Equation (3.16) and sequentially the second from Equation (3.23).

If all the coefficients must be determined in this manner, the predictive ability of the model is greatly reduced. For each coefficient which may be determined independent of concentration data, the predictive capacity increases one degree. In the example of the dissolved oxygen deficit, all of the coefficients are known at least in order of magnitude and a more exact value is specified by analysis of the data. Furthermore, one of the coefficients (in this case the reaeration coefficient) may be evaluated from the hydraulic characteristics of the system, independent of the dissolved oxygen concentrations. Thus, each set of data is used to extract a value of a coefficient, but the final profile of dissolved oxygen deficit can be calculated independently. Comparison of the calculated profile to observed data indicates, first, the general validity of the model, and, second, what adjustments, if any, are required in the empirical assessment of the coefficients to achieve a closer agreement between model output and observed data.

Verification of any mathematical model is a necessity. The conceptualization of the phenomena in mathematical terms must be quantified and compared to observed data. The relative confidence in the use of the model rests on this comparison. Several difficulties arise, however, in the verification of estuarine water quality models. These include (a) gaps in available data, (b) degree of verification required, and (c) the nature of the verification. In terms of water quality, it is difficult to obtain representative data over time and space. While great strides have been made in the continuous measurement in time of certain variables such as DO, temperature, and conductivity, it should be noted that these are point measurements. The adequate determination of spatial detail is required. Continuous recording of other variables such as coliform bacteria, chlorophyll, algae, or various pesticides is not available. There are therefore many problem areas especially in estuarine situations where only grab sample data are available. In terms of utilizing mathematical models, all data (assuming it is accurately measured) is of some use. However, data availability governs, to a large extent, the extent of the verification that is possible.

Given these data difficulties, present model verification consists essentially of judgmental comparisons between observed and computed data. This comparison should be conducted for a variety of combinations of freshwater flow, waste water inputs and temperature. Where possible, "independent" verifications are carried out in the sense that the system parameters used for one verification are subsequently used to compare observed and computed data for a second set of survey data. This process is continued until a "consistent" set of system parameters is obtained. The determination of the reasonableness of the "fit" is left to the analyst. The state of the art has not yet progressed to the point where rigorous statistical comparisons are made between observed and computed data. This is primarily due to the relative uncertainty of the observed data itself. For example, in the one dimensional models discussed previously, homogeneity is assumed in the cross section. Data collected during a survey must be related to the total cross-section, and the variability in the observed data must be taken into account. This is especially significant for estuaries where the tidal oscillations occur and where the variability of models in use refer to average tidal conditions. In other words, observed data are only estimates of the "true" nature of the water quality variable. In some cases, the observed data are only very crude estimates of the "true" value and wide limits can be placed around the observed data. In the light of these difficulties in data acquisition and interpretation, present verification procedures rely heavily on the judgment of the analyst as to when a verified model has been obtained.

It should also be recognized that even with the procedure just outlined, the model has been verified only on the basis of past observed events. In that sense, the models are verified on a hindcast basis rather than a forecast basis. It is rare that one is in a situation to immediately test the ability of a model to forecast some future level of water quality given water quality levels up to the present time. The true test of the validity of a model is its ability to forecast future water quality within some acceptable limits. In large estuaries, the problem is compounded by the relatively small water quality responses expected from relatively large removals of waste. For example, in the Delaware Estuary, removals of 100,000 lbs of BOD per day are estimated to result in DO improvements of about 0.5 mg/l in the lower part of the estuary. The determination of whether, in fact, 0.5 mg/l improvement occurred after removal of 100,000 lbs/day is difficult and requires an extensive sampling program.

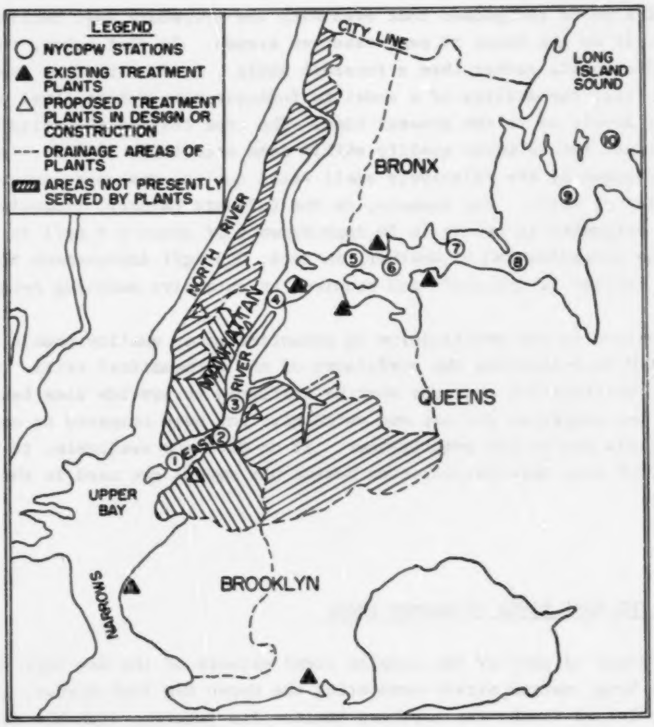
These problems in the verification of estuarine water quality models must be recognized and appreciated in evaluating the usefulness of any mathematical trial. Notwithstanding all these problems, verification analyses must be performed to provide some basis for prediction. Models that are suggested for use and which have not been compared to observed data at any level are of little use to the practitioner. If no data are available, it behooves the analyst to insist that some data be collected before his models are used in the water quality improvement program.

6.1 AN EXAMPLE: THE EAST RIVER (O'Connor 1966)

The East River is part of the complex tidal network of the New York metropolitan area. It is essentially a long, narrow strait connecting the Upper New York Harbor, its southern boundary, with Long Island South, its northern limit. Its junction with the Harlem River is located approximately midway between these points. It receives no freshwater flow except for the waste waters and the periodic storm overflows. These wastes contain large quantities of organic matter which cause significant depletion of dissolved oxygen. This condition is particularly acute at the end of the summer and early fall when the water temperature is maximum and a steady-state condition may be assumed.

6.1.1 Description of the System

A map of the East River showing the major elements of the system is shown in Figure 3.11. The locations of the various sources of pollution from both treated effluents and untreated waste weters are indicated. The major point sources are the existing treatment plants: Ward's Island, Bowery Bay, Tallman's Island, Hunt's Point in New York City and the City of New Rochelle. There are also a number of small plants not shown. The untreated sewage is discharged from Manhattan on the west bank and Brooklyn and Queens on the east bank. The locations of proposed treatment plants are also shown. In certain areas, the discharges contain significant quantities of industrial wastes. Harlem River and Newtown Creek, as well as the periodic discharges from storm overflows, also contribute pollutional matter to the East River. Sampling of a limited extent has indicated the presence of sludge deposits along the bed of the river. The survey stations of the New York City Department of Public Works are also indicated on Figure 3.11.



LEGEND
○ NYCDPW STATIONS
▲ EXISTING TREATMENT PLANTS
△ PROPOSED TREATMENT PLANTS IN DESIGN OR CONSTRUCTION
--- DRAINAGE AREAS OF PLANTS
▨ AREAS NOT PRESENTLY SERVED BY PLANTS
CITY LINE
LONG ISLAND SOUND
BRONX
NORTH RIVER
MANHATTAN
EAST RIVER
QUEENS
UPPER BAY
BROOKLYN
NARROWS
1
2
3
4
5
6
7
8
9
10

Fig. 3.11 Location map. Reprinted with permission from Journal Water Pollution Control Federation, Vol. 38, No. 11, Page 1814 (November, 1966), Washington, D. C. 20016.

The area of the Lower East River from the Battery to Harlem River was assumed constant, as the arithmetic average of the individual plottings taken every 500 feet. Although there is considerable variation about the mean, this assumption when incorporated in the mathematical model yielded a reasonable approximation to the observed data. The Upper East River from the Harlem River to Long Island Sound is characterized by a cross-sectional area which increases as the square of the distance from a hypothetical origin.

A schematic representation of the system is shown in Figure 3.12. A point source of pollution W at $x = a$ in the Lower East River is considered. The elements of the system for which solutions are required are designated by numerals. The solution requires the application of appropriate boundary conditions of concentration and flux to the set of equations representing each element of the system. The actual system contains the Hudson River and the Kill Van Kull. However, in order to simplify the analysis, as a first approximation the effects of these bodies are included in the freshwater flow Q and the mass input W_o. The latter term also includes the effluents from the various treatment plants which discharge directly into the harbor. Furthermore, the assumption is made that the effect of the Harlem River is not significant with respect to the BOD distribution in the East River. The flux of the East River into the Harbor is due only to diffusion, since the advective term is negligible. This contribution may be significant depending on the magnitude of the concentration gradient $d\ell_2/dx$ in the river at its confluence with the Harbor. The gradient is determined from the solution of the equation from zone II of the Lower East River and the input is equal to $EA_o\, d\ell_2/dx$ at $x = 0$. At steady state, an equilibrium concentration is achieved and the output from the system is therefore $Q\ell_1$ in which ℓ_1 equals the equilibrium concentration. When the concentration of organic matter (BOD) or any non-conservative substance is considered, a sink is the overall reaction or removal. If first-order kinetics are assumed to describe this reaction, this term is $K\ell$. Furthermore the loss from the harbor to the ocean by tidal exchange may be expressed by $R(\ell - \ell_o)$ in which R is the volumetric exchange coefficient and ℓ_o the concentration in the ocean. If the concentration in the ocean may be assumed to be zero, then the exchange may be added directly with the reaction. A summary of the equations, the boundary conditions and the general solutions for the point source is presented in Table 3.1. The constants, A_n and B_n, may be evaluated by application of the boundary conditions to the various equations.

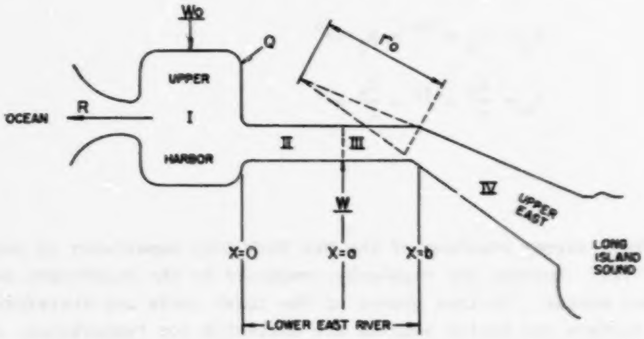


Fig. 3.12 Schematic representation of system. Reprinted with permission from Journal Water Pollution Control Federation, Vol. 38, No. 11, Page 1817 (November, 1966), Washington, D. C. 20016.

TABLE 3.1

Formulae Used in the East River Model

Zone	Equation
I	$0 = W_o + EA_o \left. \frac{d\ell_2}{dx} \right\|_{x=o} - Q\ell_1 - (K+R)V\ell_1$
II, III	$0 = E \frac{d^2\ell}{dr^2} - K\ell$
IV	$0 = E \frac{d^2\ell}{dr^2} + \frac{E}{r} \frac{d\ell}{dr} - K\ell$

Boundary Conditions

$x = \infty$	$\ell = 0$
$x = b$	$\ell_3 = \ell_4$
$r = r_o$	$\ell_3 = \ell_4$
$x = b$	$\oint j \cdot d\sigma = 0$
$x = a$	$\ell_2 = \ell_3$
$x = a$	$\oint j \cdot d\sigma = W$
$x = 0$	$\ell_1 = \ell_2$

Zone	General Solutions
I	$\ell_1 = \left(W_o + EA_o\,(-jA_2 + jB_2)\right) \Big/ \left(Q + (K+R)\,V\right)$
II	$\ell_2 = A_2\, e^{-jx} + B_2\, e^{jx}$
III	$\ell_3 = A_3\, e^{-jx} + B_3\, e^{jx}$
IV	$\ell_4 = \frac{A_4}{r}\, e^{-jr} + \frac{B_4}{r}\, e^{jr}$

6.1.2 Field Data

The East River survey stations of the New York City Department of Public Works are indicated in Figure 3.11. Surveys are regularly conducted by the Department once or twice a week during the summer months. Various phases of the tidal cycle are therefore encountered at each station. Both surface and bottom samples are collected for temperature, dissolved oxygen, chlorides, biochemical oxygen demand and coliform bacteria. A typical set of data of both surface and bottom samples is shown on Figure 3.13. The broken lines are drawn through the data to indicate the trend, rather than a functional relationship. Vertical stratification in temperature and concentration may be observed. This characteristic is particularly

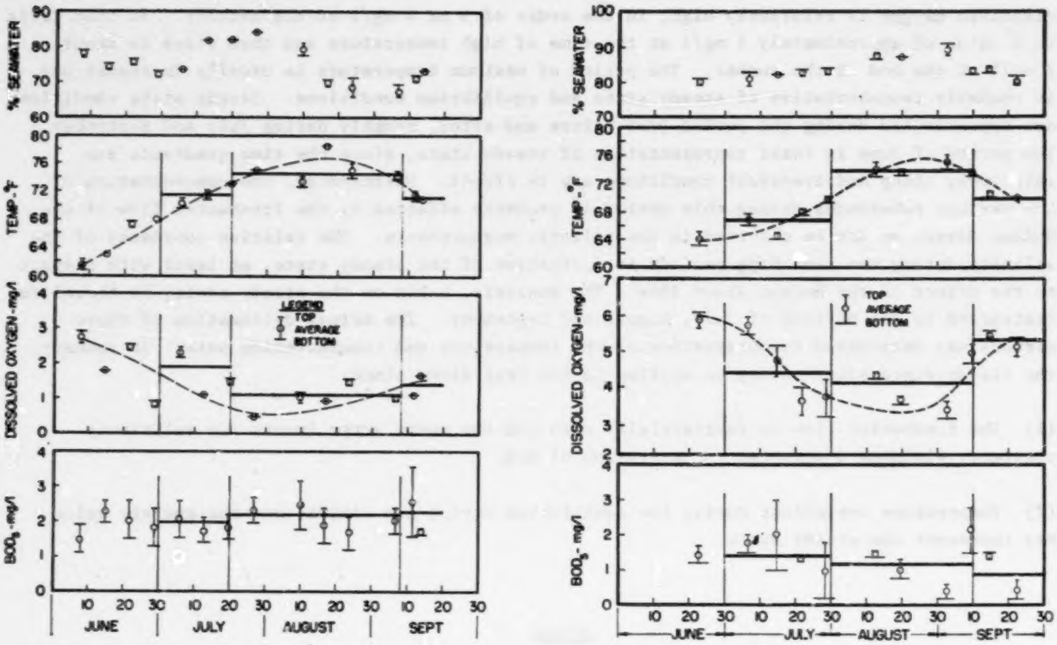


Fig. 3.13 Variation of water characteristics. Left: Lower East River, 23rd St., Station E-2, 1955. Right: Upper East River, Hart's Island, Station E-10, 1959. Reprinted with permission from Journal Water Pollution Control Federation, Vol. 38, No. 11, Page 1823 (November, 1966), Washington, D. C. 20016.

noticeable in the BOD concentration. The difference between top and bottom salinities and temperatures, although consistent, is minimal, i.e., the maximum temperature and the minimum salinity are always measured in the surface samples, but the order of magnitude of the difference is low. Although the dissolved oxygen concentration of the surface samples is usually greater by about 0.2 or 0.3 mg/l than that of bottom samples, the difference is not consistent. In many cases, higher concentrations are observed in the bottom samples. Vertical uniformity is therefore assumed as a condition for the analysis as a first approximation.

6.1.3 Analysis of Data

It may be observed from these data that the concentration of the biochemical oxygen demand is fairly constant over the summer. This observation is consistent with the zero freshwater flow and a constant rate of waste water discharge. From these data it may be assumed that the BOD distribution has achieved steady state and is in equilibrium, the temperature variations having a minor influence on the concentration. However, the effect of the time-varying temperature on the dissolved oxygen concentration is marked. Maximum water temperatures are coincident with minimum dissolved oxygen concentrations, which usually occur in late July, August or early September. The earliest measurements are taken in June, when the dissolved oxygen is relatively high, in the order of 3 or 4 mg/l at the Battery. It then falls to a value of approximately 1 mg/l at the time of high temperature and then rises to about 2 mg/l at the end of the summer. The period of maximum temperature is usually in August and is probably representative of steady-state and equilibrium conditions. Steady-state conditions are approximated during the period just before and after, roughly during July and September. The period of June is least representative of steady state, since the time gradients are relatively steep and transient conditions are in effect. Furthermore, the concentration of the various substances during this period is probably affected by the freshwater flow of the Hudson River, as may be observed in the salinity measurements. The relative constancy of the salinity during the remaining periods is indicative of the steady state, at least with respect to the effect of the Hudson River flow. The analysis, based on the steady state, is therefore restricted to the periods of July, August and September. The actual delineation of these periods was determined by observation of the temperature and concentration data. In summary, the steady-state solution may be applied to the East River since:

(1) The freshwater flow is substantially zero and the waste water inputs are relatively constant, yielding a constant concentration of BOD.

(2) Temperature variations during the equilibrium period are minimal and the average value may represent the steady state.

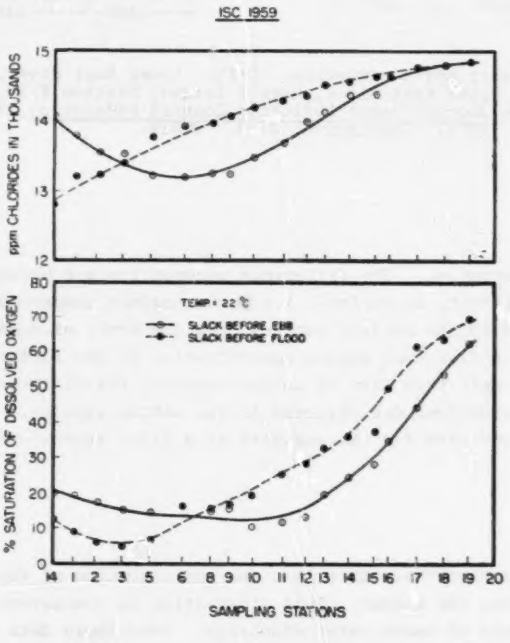


Fig. 3.14 Spatial distribution of chlorides and DO at slack water. Reprinted with permission from Journal Water Pollution Control Federation, Vol. 38, No. 11, Page 1824 (November, 1966), Washington, D. C. 20016.

(3) Tidal variations are eliminated by considering slack water measurements or average values over a significant period, as described above.

The individual data shown in these figures are based on samples taken at various times over the tidal cycle and therefore reflect the effect of tidal translation. This factor accounts, in large measure, for the deviations of the observed data from the average trend. The tidal effect is well borne out by the data collected by the Interstate Sanitation Commission in the summer of 1959, during which period a short-term, intensive survey was conducted. Dissolved oxygen, temperature and salinity were measured hourly every day for a three-week period. The spatial distribution of the average values at high and low water slack are shown in Figure 3.14. The variation over the tidal cycle is minimal in the vicinity of the low point on the DO profile where the gradient is flat, but significant in portions of the Upper East River where the gradient is steep. A typical set of spatial DO data for one season is shown in Figure 3.15.

6.1.4 Waste Water Discharges

The BOD input data from the treatment plant effluents and average water temperatures are given in Table 3.2 for the month of July, 1960, the period selected for analysis.

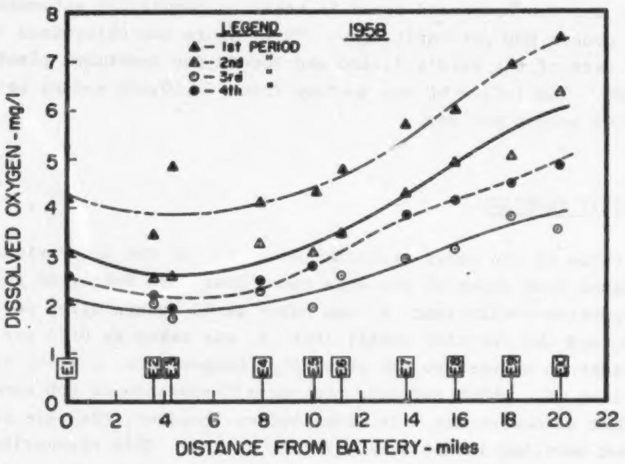


Fig. 3.15 Spatial distribution of DO over summer period. Reprinted with permission from Journal Water Pollution Control Federation, Vol. 38, No. 11, Page 1825 (November, 1966), Washington, D. C. 20016.

TABLE 3.2

TREATED BOD SOURCES

Treated Point Sources	Pounds Per Day
Ward's Island	37,600
Bowery Bay	50,000
Hunt's Point	14,700
Tallmans Island	5,600

UNTREATED BOD SOURCES

Distributed Sources	Pounds per Day - Mile	Distance (Miles)
Manhattan	14,200	7.0
Brooklyn-Queens	17,900	5.2
Storm Overflows	7.5% of the total BOD from drainage areas receiving treatment	
Newtown Creek	30,600	
Harlem River	6,600	

Average Water Temperature 22°C

The BOD input for the untreated areas is based on population estimates, assuming a unit discharge of 0.17 pounds BOD per capita-day. This figure was determined from an average of the July and August data of the Ward's Island and Bowery Bay treatment plants for the period from 1956 to 1960. The influx of the Newtown Creek is 30,600 pounds per day, and of the Harlem River is 6,600 pounds per day.

6.1.5 BOD AND DO DEFICIT PROFILES

The average value of the cross-sectional area A_o of the lower river is 80,000 square feet, which was determined from plots of the area taken every 500 feet from the Battery to the Harlem River. The dispersion coefficient E was taken as 10 square miles per day for all elements of the system, and the reaction coefficient K was taken as 0.23 per day at 20°C for all sources. In order to convert to the prevailing temperature, a value of 1.04 for θ was used. The coefficient K, which reflects the overall reaction of BOD removal, is not necessarily equal to that of deaeration. In tidal bodies, however, they are usually of the same magnitude, provided settling is not a significant factor. This assumption is made in this analysis. An example of the individual profiles and the total profile of BOD is shown in Figure 3.16 with the observed 5-day BOD values for the period of July 1960. Dividing this value by the bottom area-volume ratio yields a numerical value of 0.18 mg-day/l.

An approximate value of the reaeration coefficient K_2 was calculated by the formula

$$K_2 = \frac{D_2 U_o^{1/2}}{H^{3/2}}$$

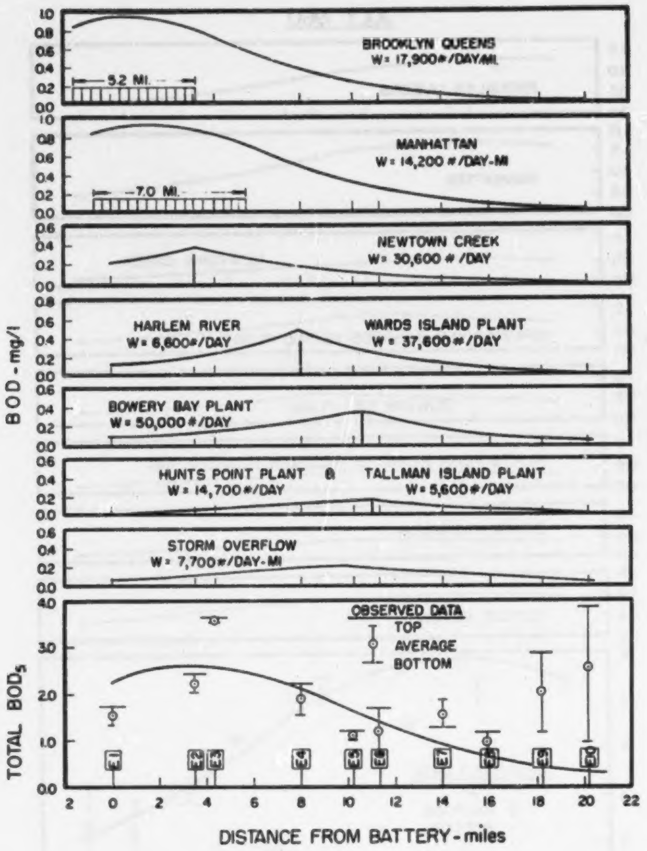


Fig. 3.16 Individual and total BOD profiles. Reprinted with permission from Journal Water Pollution Control Federation, Vol. 38, No. 11, Page 1827 (November, 1966), Washington, D. C. 20016.

in which D_2 = coefficient of diffusivity of oxygen in water

U_o = average tidal velocity

H = average depth.

The average tidal velocity is the mean between the average ebb and flood tide for the lower and upper sections. The average depth was determined from the cross-sectional area data. Values of this coefficient at 20° are 0.08 per day and 0.11 per day for the lower and upper rivers respectively. In order to convert to the prevailing temperature, the value of the coefficient θ was taken as 1.02. Samples of the individual DO deficit profiles and the total deficit profile for the period of July 1960 is shown in Figure 3.17. These profiles of DO deficit and BOD are typical. In general the deficit profile is a better fit than that of the BOD, particularly in the upper East.

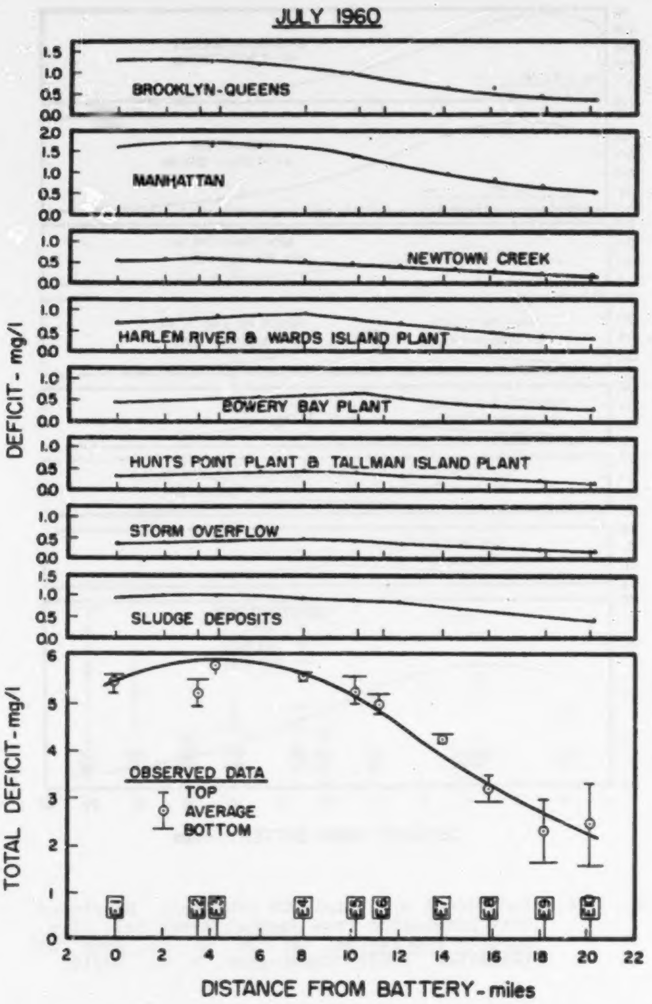


Fig. 3.17 Individual and total DO deficit profiles. Reprinted with permission from Journal Water Pollution Control Federation, Vol. 38, No. 11, Page 1828 (November, 1966), Washington, D. C. 20016.

6.1.6 Discussion

The distribution among the carbonaceous matter, nitrogenous material, storm overflows and sludge deposits should be determined in each estuarine analysis. The relative contribution of each of these factors is significant, not only with regard to present water quality, but more important, to future conditions when treatment facilities are installed. Treated effluents may have a more pronounced effect on the oxygen resources of the system than has been appreciated. Although the carbonaceous matter is effectively removed in high rate biological treatment plants, the nitrogenous components of this material may pass through relatively unaffected. This condition gives rise to an environment which is conducive to the growth and development of the nitrifying bacteria. The effect of nitrification is apparently not as pronounced in the untreated discharges. Thus, that portion of the dissolved oxygen depression which is the result of nitrification under present conditions of little or no treatment, may be much more significant under future conditions of partial or secondary treatment. It is most important that the relative effects of each component in both raw and treated effluents be more fully investigated and assessed.

7. FUTURE DIRECTIONS

7.1 STEADY-STATE FEEDBACK MODELING

There are several phenomena in water quality problems that are characterized by "feedback" effects. Examples include the loss of nutrient material to sediments with subsequent feedback into the overlying water, and the utilization of nutrients by algae with subsequent release of the nutrients upon algal death. Figure 3.18 shows the major features of the nitrogen cycle and indicates several possible feedback loops. This figure can be compared to Figure 3.4 which illustrated only the feedforward phenomena of nitrification with accompanying oxygen utilization. Section 2.6 discussed the importance of the nitrogen component of waste discharges.

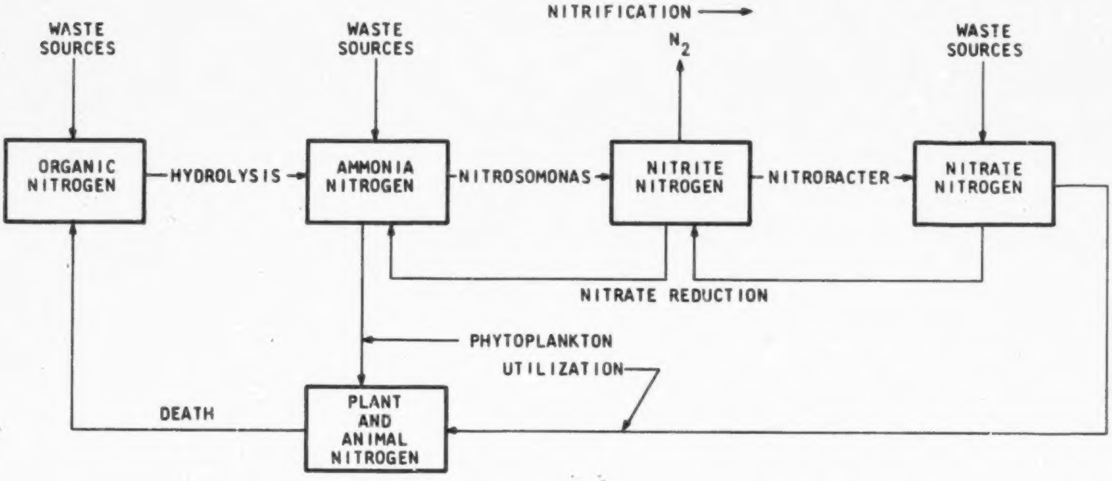

NITRIFICATION
WASTE SOURCES
WASTE SOURCES
N_2
WASTE SOURCES
ORGANIC NITROGEN
HYDROLYSIS
AMMONIA NITROGEN
NITROSOMONAS
NITRITE NITROGEN
NITROBACTER
NITRATE NITROGEN
NITRATE REDUCTION
PHYTOPLANKTON
UTILIZATION
DEATH
PLANT AND ANIMAL NITROGEN

Fig. 3.18 Major features of the nitrogen cycle.

For some problem situations, then, it is useful to have available a generalized steady-state model which can incorporate feedback (or feedforward) loops in a multi-dimensional water body with N consecutive reactions. For preliminary studies to determine general order-of-magnitude responses, such a model provides the user with the ability to analyze any system configuration. The model therefore represents the limit of complexity of estuarine models under steady-state and first-order kinetics assumptions.

The use of the finite section (difference) approach for consecutive reactions was given previously in matrix form in Section 3.3. In addition, it was shown in Section 4 that in principle the addition of lateral or vertical water quality gradients results in a general matrix of coefficients rather than the tridiagonal form as for one-dimensional estuaries. All that remains is to incorporate any first-order kinetic feedback loop from any substance in the consecutive reaction sequence to any other substance. A complete description of the model is given in Manhattan College (1970).

The matrix equations with all feedforward and feedback loops are then given by

$$
\begin{aligned}
\left[A^1\right]\left(c^1\right) &= \left(W^1\right) + \left[VK^{21}\right]\left(c^2\right) + \left[VK^{31}\right]\left(c^3\right) + \ldots \left[VK^{N1}\right]\left(c^N\right) \\
\left[A^2\right]\left(c^2\right) &= \left(W^2\right) + \left[VK^{12}\right]\left(c^1\right) + \left[VK^{32}\right]\left(c^3\right) + \ldots \left[VK^{N2}\right]\left(c^N\right) \\
&\vdots \\
\left[A^i\right]\left(c^i\right) &= \left(W^i\right) + \left[VK^{1i}\right]\left(c^1\right) + \left[VK^{2i}\right]\left(c^2\right) + \ldots + \left[VK^{i+1,i}\right]\left(c^{i+1}\right) + \ldots \left[VK^{Ni}\right]\left(c^N\right) \\
&\vdots \\
\left[A^N\right]\left(c^N\right) &= \left(W^N\right) + \left[VK^{1N}\right]\left(c^1\right) + \ldots + \left[VK^{N-1,N}\right]\left(c^{N-1}\right)
\end{aligned}
\tag{3.58}
$$

As before, the matrices $[A^i]$ are of size $n \times n$ where n is the number of spatial segments. The superscript i refers to the i^{th} substance in an N-stage consecutive reaction sequence. The matrices $[A^i]$ differ only in the K_{ii} on the main diagonal. The vector (c^i) is an $n \times 1$ vector representing the spatial distribution of the output of the i^{th} reaction; $[VK^{ij}]$, $i < j$, represents the feedforward loops as an $n \times n$ diagonal matrix and $[VK^{ij}]$, $i > j$, represents the feedback loops, both given by the vector of first-order reaction coefficients (K); and (W^i) is an $n \times 1$ vector of input of waste material of the i^{th} reaction.

In matrix form, the matrix equations (3.58) can be written

$$
\begin{bmatrix}
\left[A^1\right] & \left[-VK^{21}\right] & \ldots & \left[-VK^{N1}\right] \\
\left[-VK^{12}\right] & \left[A^2\right] & \ldots & \left[-VK^{N2}\right] \\
\vdots & \vdots & & \vdots \\
\left[-VK^{1N}\right] & \left[-VK^{2N}\right] & \ldots & \left[A^N\right]
\end{bmatrix}
\begin{pmatrix} c^1 \\ c^2 \\ \vdots \\ c^N \end{pmatrix}
=
\begin{pmatrix} W^1 \\ W^2 \\ \vdots \\ W^N \end{pmatrix}
\tag{3.59}
$$

or

$$
\left[\hat{a}\right]\left(\hat{c}\right) = \left(\hat{W}\right) \tag{3.60}
$$

where $[\hat{a}]$ is an $nN \times nN$ matrix, $(\hat{c})$ is an $nN \times 1$ solution vector and $(\hat{W})$ is an $nN \times 1$ waste load input vector. The solution vector is given formally by

$$(\hat{c}) = [\hat{a}]^{-1} (\hat{W}) \tag{3.61}$$

The steady-state multi-dimensional, N reaction system with any feedback-feedforward configuration water quality problem is therefore given by solution of Nn equations or inverting matrix $[\hat{a}]$ as given by Equation (3.61). This approach can be quite useful for a variety of water quality problems providing one is willing to accept first-order kinetics. Although the solution technique is computationally direct (e.g. matrix inversion or solution of simultaneous equations) special care must be taken in computer algorithms to ensure proper problem set-up and data input preparation. A Gauss-Seidel relaxation technique is used for simultaneous solution of the equations with generation of the matrix inverse as an option.

The steady-state feedback model was used in a preliminary analysis of steady-state water quality profiles in the Potomac Estuary (Thomann et al. 1970). The objective of the analysis was to obtain greater insight into the effect of feedback and to determine the usefulness of the approach in sequential reactions such as nitrification.

The major waste source in the Potomac Estuary is the effluent of the Washington, D. C. secondary waste treatment plant. Water quality problems include low DO in the vicinity of the District of Columbia discharge and high algal concentrations downstream. A steady-state feedback model which considers organic, ammonia and nitrate nitrogen forms was constructed. A feedback loop is incorporated which represents ammonia and nitrate nitrogen utilization by algae with the subsequent nitrogen release upon death recycled to the organic nitrogen form. The loop therefore represents the utilization of nitrogen by algae with subsequent nitrogen release upon death. The four system model (organic, ammonia, nitrate and nitrogen found in living algae) can therefore be used to obtain information on the behavior of the nitrogen cycle in the Potomac. Figure 3.19 shows the results of an analysis of data collected during July - August 1968.

The first-order reaction coefficients for the verification analysis shown in Figure 3.19 are given in Table 3.3.

TABLE 3.3

Reaction Coefficients - Potomac Estuary, July-August 1968

Temperature = 28°C

Nitrogen Step	Reaction Coef (1/day)	Nitrogen Step	Reaction Coef (1/day)
Decay of Organic-N	0.1		
Organic-N → NH_3-N	0.1	NO_3-N → Algal-N	0.1
NH_3-N → NO_3-N	0.28	Algal-N → Organic-N	0.12
NH_3-N → Algal-N	0.02		

These coefficients represent the end result of many runs which tested the effects of various interactions and levels of coefficients. There is no a priori reason for assuming this set of coefficients to be unique. The order of the reaction rates is, however, similar to that which

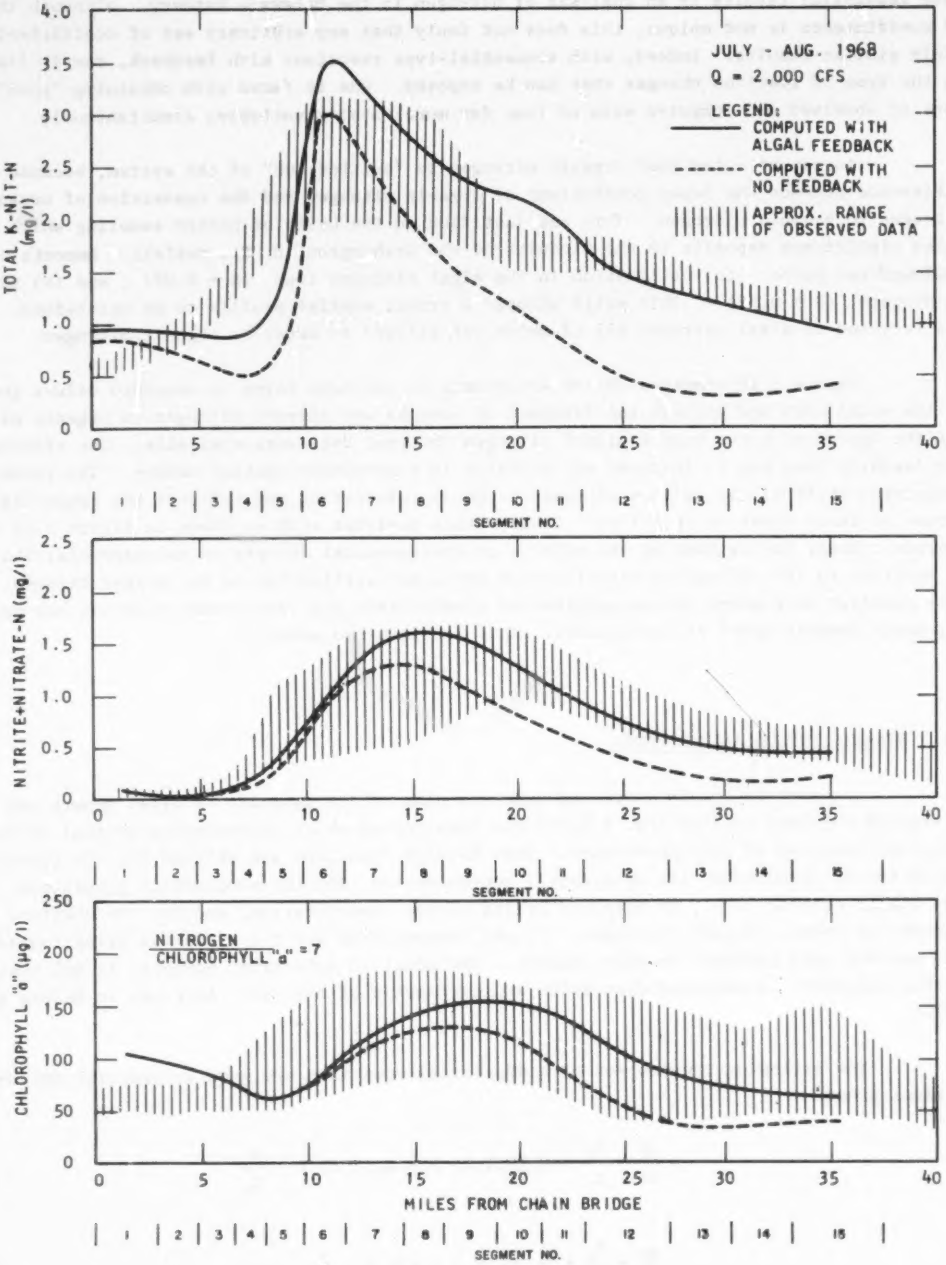


Fig. 3.19 Comparison of observed and computed (solid lines) nitrogen and chlorophyll - Potomac Estuary, July-Aug. 1968.

gave meaningful results in an analysis of nitrogen in the Delaware Estuary. Although the set of coefficients is not unique, this does not imply that any arbitrary set of coefficients will yield similar results. Indeed, with sequential-type reactions with feedback, one is limited in the type of reaction changes that can be imposed. One is faced with obtaining "good" agreement of observed and computed data of four (or more) system variables simultaneously.

It can be noted that organic nitrogen is "settled out" of the system, because of the difference between the decay coefficient of organic nitrogen and the conversion of organic nitrogen to ammonia nitrogen. This was justified on the basis of bottom sampling which indicated significant deposits in the vicinity of the Washington, D. C., outfall. Ammonia nitrogen followed two paths: (a) utilization in the algal nitrogen loop $(K = 0.02)$, and (b) oxidation to nitrate $(K = 0.28)$. This split allowed a proper spatial profile to be maintained. Nitrate was recycled to algal nitrogen all of which was allowed to decay to organic nitrogen.

Figure 3.19 compares the observed data on nitrogen forms to computed values generated by the model with and without the feedback of ammonia and nitrate nitrogen to organic nitrogen. For the uppermost curve only Kjeldahl nitrogen observed data were available. The effects of the feedback loop are to increase all profiles in a nonlinear spatial manner. The relative downstream shift of the various nitrogen forms is interesting and reflects the sequential nature of these types of reactions. Steady-state analyses such as shown in Figure 3.19 can provide a basis for estimating the effects of environmental changes on nitrogen distribution in addition to the effects of nitrification and algal utilization on the oxygen regimes. For more detailed work where the assumptions of steady-state and first-order kinetics are dropped, a general dynamic model is appropriate. This is discussed below.

7.2 DYNAMIC PHYTOPLANKTON MODEL

In order to obtain increased understanding of the dynamics of algal growth and subsequent nutrient utilization, a model was constructed which incorporates several of the important features of this phenomenon. Mass balance equations are written for the phytoplankton population as measured by its chlorophyll concentration, for the zooplankton population, the next higher trophic level, as measured by its carbon concentration, and for the nutrient level as measured by total inorganic nitrogen. It was assumed that for the situation being considered this was the only nutrient in short supply. The model in principle, however, is not restricted to this nutrient. A detailed discussion and derivation of the model is given in DiToro et al. (1970).

The following coupled set of differential equations are used to describe the dynamics of algal growth:

$$\frac{dP}{dt} = \frac{P_s}{t_o} + G_p(N,I,T)\ P - D_p(Z,T)\ P - \frac{P}{t_o} \qquad (3.62)$$

$$\frac{dZ}{dt} = \frac{Z_s}{t_o} + G_z(P)\ Z - D_z(T)\ Z - \frac{Z}{t_o} \qquad (3.63)$$

$$\frac{dN}{dt} = \frac{N_s}{t_o} - b\ G_p(N,I,T)\ P + S(P,Z,T) - \frac{N}{t_o} + \frac{W}{V} \qquad (3.64)$$

where P is phytoplankton chlorophyll, $G_p(N,I,T)$ is the phytoplankton growth rate as a function of inorganic nitrogen concentration (N), solar radiation (I) and temperature (T); $D_p(Z,T)$ is the death rate of phytoplankton due to zooplankton (Z) grazing and endogenous respiration; Z is the zooplankton concentration; G_z and D_z are zooplankton growth and death rates, respectively; b is the nitrogen yield coefficient (mass nitrogen/mass algae) and W is the input nitrogen from waste discharges or land runoff. A schematic of the type of system under investigation is shown in Figure 3.20. The form given in Equations (3.62) - (3.64) corresponds to a completely mixed water system with t_o as the detention time, equal to the volume divided by the flow, and P_s, Z_s and N_s are respective influent concentration. For situations where spatial gradients exist, additional terms are necessary to incorporate the advection and tidal dispersion. However, the incorporation of spatial gradients does not alter the conceptual model of the dynamics of the system, but it does increase computational complexity.

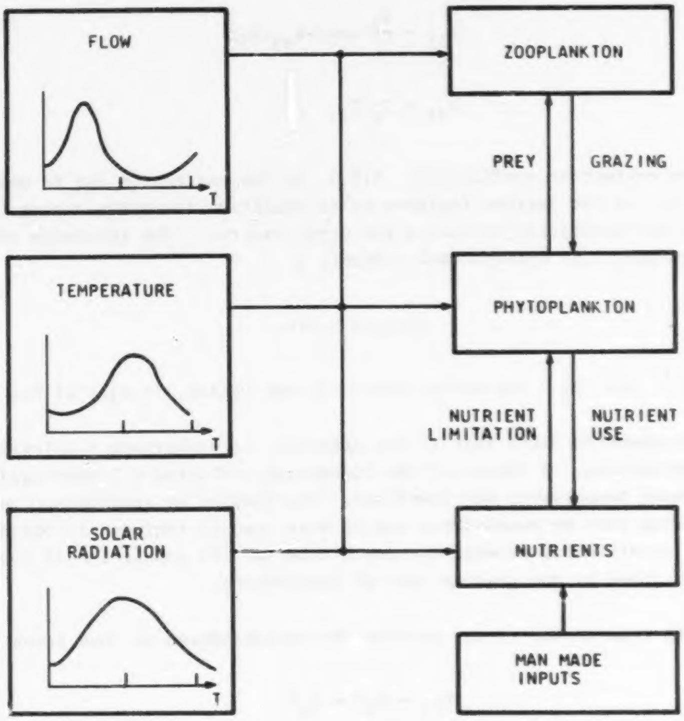

FLOW
T
TEMPERATURE
T
SOLAR RADIATION
T
ZOOPLANKTON
PREY
GRAZING
PHYTOPLANKTON
NUTRIENT LIMITATION
NUTRIENT USE
NUTRIENTS
MAN MADE INPUTS

Fig. 3.20 Interactions: environmental variables and the phytoplankton, zooplankton, and nutrient systems.

In any application, the general expressions for the growth and death coefficients must be made explicit. Phenomena such as nonlinear growth as a function of nutrient concentrations (using Michaelis-Menten expressions) and solar radiation, light extinction, self-shading, and temperature are included in the growth and death terms for phytoplankton. For the case of one limiting nutrient, say total inorganic nitrogen, the growth expression for the rate in the j th segment of the water body is given by

$$G_{pj} = K_1 T_j \left[\frac{2.718f}{k_{ej} H_j}\left(e^{-\alpha_{1j}} - e^{-\alpha_{oj}}\right)\right] \frac{N_j}{K_m + N_j} \tag{3.65}$$

Here K_1 is the saturated growth rate of phytoplankton, T_j is water temperature, H_j is water depth, f is the photoperiod, N_j is total inorganic nitrogen concentration, K_m is the Michaelis constant for total inorganic nitrogen and

$$k_{ej} = k'_{ej} + h(P_j)$$

$$\alpha_{1j} = \frac{I_a}{I_s} \exp(-k_{ej} \cdot H_j)$$

$$\alpha_{oj} = I_a / I_s$$

where k'_{ej} is the extinction coefficient, $h(P_j)$ is the extinction due to phytoplankton (self-shading), I_a is the average incident solar radiation intensity during the photoperiod and I_s is the light saturation intensity for phytoplankton. The inclusion of the self-shading phenomena $h(P_j)$ is incorporated linearly as

$$h(P_j) = 0.17P_j$$

for h in meters^{-1} and P_j , the phytoplankton concentration, in mg/l of dry weight.

The phytoplankton death rate is due primarily to endogenous respiration and grazing by herbivorous zooplankton.* A search of the literature indicated a linear equation between respiration and water temperature was justified. The grazing by zooplankton requires a knowledge of the filtering rate by zooplankton and is most readily included in the death rate by assuming a direct relationship between the death rate and the population of zooplankton. The proportionality is given by the grazing rate of zooplankton.

The death rate in the j th section for phytoplankton is thus given by

$$D_{pj} = K_2 T + C_g Z_j \tag{3.66}$$

Incorporation of the growth rate, Equation (3.65), and death rate, Equation (3.66), into the phytoplankton growth equation (3.62) completes that equation in terms of the primary variables, light, temperature, nutrient concentrations and zooplankton. However, the nutrient and zooplankton concentrations must be obtained simultaneously in order to solve the entire interdependent system given by Equations (3.62) to (3.64).

For the zooplankton system, the source of zooplankton biomass is

$$S_{zj} = (G_{zj} - D_{zj})Z_j$$

where G_{zj} and D_{zj} have units of day^{-1}, and Z_j is the concentration of zooplankton carbon in volume element V_j. The growth rate G_{zj} is a function of the phytoplankton concentration, since at high phytoplankton counts the zooplankton do not metabolize all the phytoplankton that they graze, but rather excrete a portion of the phytoplankton in undigested or semi-digested form. A convenient choice for a functional relationship is a Michaelis-Menten form, so that the growth rate for zooplankton is given by

$$G_{zj} = A_{zp} C_g K_{mp} \left(\frac{P_j}{K_{mp}+P_j}\right)$$

where A_{zp} is the utilization efficiency which relates phytoplankton biomass ingested to zooplankton biomass produced (approximately 0.6), C_g is the filtering rate, and K_{mp} is the Michaelis constant, set at 60μg chlorophyll/liter in this work.

The death rate for zooplankton depends on both predation by higher trophic levels and endogenous respiration. In this model, the death rate was given by

$$D_{zj} = K_3 T + K_4$$

where K_4 is an empirically determined constant.

The nutrient system can now be readily written down since the sink term for phytoplankton, zooplankton excretion and mortality sources have been formulated. In addition to these sources and sinks of total inorganic nitrogen, the direct sources W as shown in Equations (3.64) must also be included. Thus the net source-sink term for nitrogen is

$$(S_{net})_j = \frac{W_{Nj}}{V_j} - b\ G_{Pj}P_j + b\ C_g Z_j P_j \left[1 - \frac{A_{zp}K_{mp}}{K_{mp}+P_j}\right] \qquad (3.67)$$

$$+ b\ K_2 T P_j + A_{nz} K_3 T Z_j$$

All growth, death and source-sink terms have now been formulated. It should be noted that although the expressions all include various coefficients, the literature provides laboratory and/or field estimates for the majority of the parameters. Indeed in the application of the model all the parameters were required to vary only within reported literature values.

The equations discussed above were applied to phytoplankton and zooplankton populations observed at Mossdale Bridge on the San Joaquin River in California during the two years 1966 and 1967. The San Joaquin River, located in the center of Western California, in the vicinity of its confluence with the Sacramento River, forms a delta which is an extremely productive agricultural region. The combined discharge from these rivers flows through the Delta network, Suisun and San Pablo Bays through the North San Francisco Bay and then to the ocean.

For an initial application of the nonsteady-state algal growth model, the region near Mossdale was selected. This location is on the San Joaquin River, about thirty miles from its confluence with the Sacramento. The river in this region is quite shallow and although it is turbid, the region is nevertheless productive. For simplicity, a reach of the San Joaquin in the vicinity of Mossdale was considered to be a completely mixed system.

The solution to Equations (3.62) - (3.64) with nonlinear time-variable coefficients as given in Equations (3.65) - (3.67) requires machine computation. For this study, the equations were integrated on an IBM 1130 computer using a Continuous System Modeling Program (CSMP). This software package incorporates a system simulation language which allows the user to specify equivalent analog components which are then implemented digitally. Time-variable solar radiation, inflows, temperature and concentration inputs can all be handled in this manner. At each integration step, the equations are integrated numerically using a second-order Runge-Kutta approximation. In this approximation, a half-step integration is performed to give

$$y^*_{\frac{1}{2}} = y_o + \frac{h}{2} f(t_o, y_o)$$

and this value of y is used to estimate the slope at the midpoint of the interval which is then used as the slope of the straight-line approximation

$$y_1 = y_o + hf(t_o + \frac{h}{2}, y^*_{\frac{1}{2}})$$

The environmental variables used as input for the two-year period of interest and the straight-line approximations used in the numerical computations are shown in Figure 3.21. A comparison between observed data over two years (1966-67) and the calculated solution is shown in Figure 3.22. The growth and death coefficients in Equations (3.65) - (3.67) were computed internally as nonlinear functions of temperature, nutrient concentrations, and light, using the appropriate functional forms. Net growth rates (growth minus predation and death) contributing to exponential phytoplankton growth during the spring varied from 0.0 to about 0.3/day. The various coefficients and parameters in the equations were then adjusted to achieve an acceptable fit of the data. However, in no case did the assigned values for the coefficients exceed the boundaries of reported levels. There is a marked difference in the phytoplankton population which developed during the two years. In 1966 a large population formed in the spring, thereby reducing the inorganic nitrogen concentration markedly. This population then remained stable throughout the summer and fall. By contrast in 1967, no significant population developed during the spring and summer, and not until the late fall did a population begin to develop. The cause for the differences in these two years is due to the variation in hydrographs. In the spring and summer of 1967, the freshwater flow was very large resulting in a wash-out of the population during this period. Only during the late fall did the flow decrease sufficiently so that a population could develop. The model calculations behave in a similar way and the agreement obtained is quite encouraging.

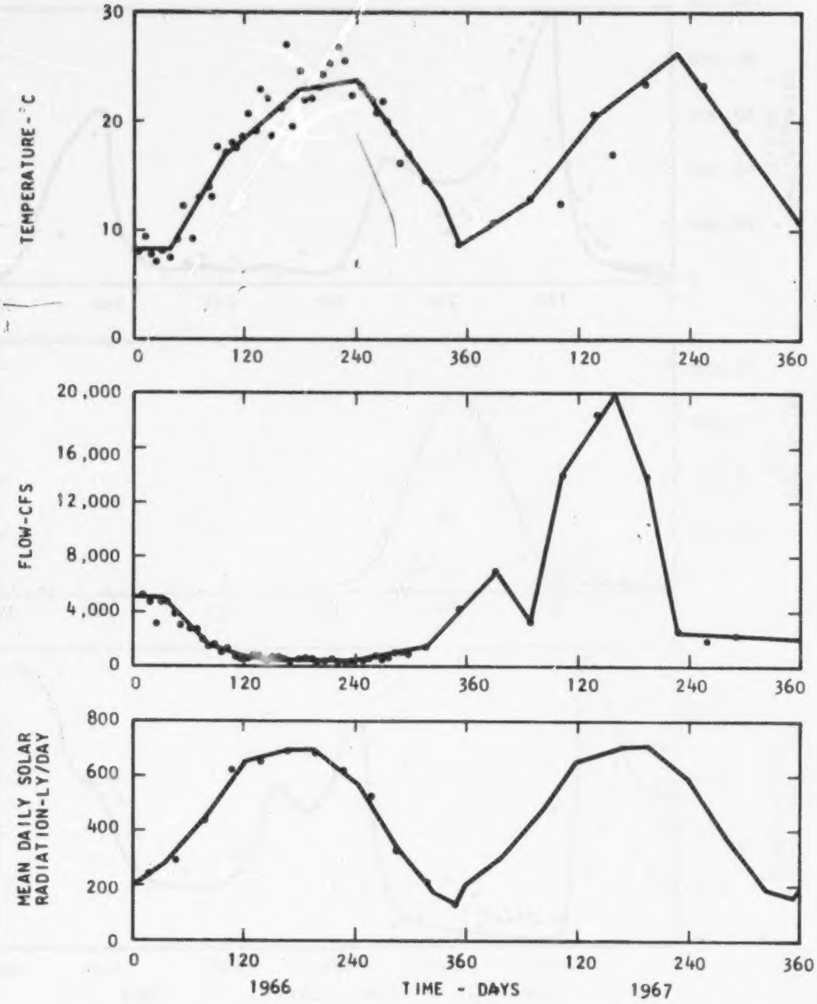


Fig. 3.21 Temperature, flow and mean daily solar radiation. San Joaquin River, Mossdale, 1966-1967.

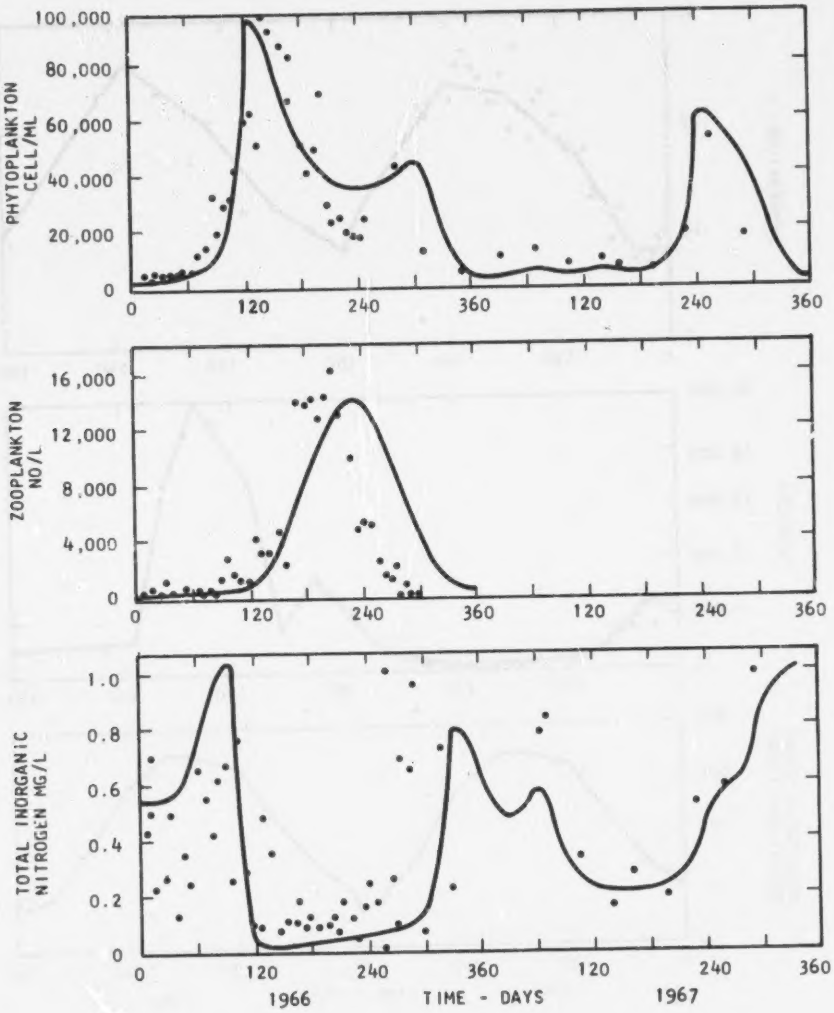


Fig. 3.22 Phytoplankton, zooplankton, and total inorganic nitrogen. Comparison of theoretical calculations and observed data. San Joaquin River, Mossdale, 1966-1967.

8. DISCUSSION AND RECOMMENDATIONS

On the basis of the quality models outlined in the preceding sections of this chapter, it is appropriate to compare and contrast, in a general manner, hydrodynamic and quality modeling. In a fundamental sense, both utilize the same basic principles of conservation of mass. The distinction between the two modeling efforts lies in the fact that the principles and mechanisms which underly most hydrodynamic phenomena are reasonably well understood and quantified. The mathematical relationships which describe the hydrodynamics of a system are scientifically more valid than those which are used to describe most biological and some chemical reactions in natural waters. (Note, for example, that in all three sections of Chapter II, one can immediately write down the equations of motion as a starting point. Such is not the case with water quality problem contexts where the phenomenon itself is not yet clear.) The nature of these biological and chemical phenomena are known, in a qualitative fashion, but in most cases have not been described in a quantitative manner. In the case of some simple, single-stage reactions, significant progress has been made and fundamental relationships are available, comparable to those in the hydrodynamic realm.

However, in the case of consecutive, complex reactions, which are more relevant to water quality problems, the relationships are not available and mathematical simplifications are therefore assumed in order to make the equations more tractable. While the assumed relations are effective in fitting prototype observations, it is recognized that they may not be fundamental, and they are utilized more for their simplicity than their validity.

Furthermore, historical data of water quality, particularly of a biological nature, is generally less available than that of hydrodynamic observations such as tides and currents in estuaries and bays. This lack of quality data imposes further restrictions on the extent to which water quality modeling can be developed. In view of these factors, it must be accepted that quality modeling is greatly restricted by contrast to hydrodynamic modeling. One of the most difficult assessments to make in this regard, therefore, is the extent to which the more advanced hydrodynamic modeling should be incorporated in the less sophisticated quality modeling. Part of the answer is found in applying the criteria described in the beginning of this chapter, particularly with respect to appropriate time and space scales. In general, hydrodynamic developments should be incorporated to a level of significance with respect to the water quality problem under investigation and not beyond. More advanced hydrodynamic modeling offers no further advantage from the quality viewpoint. This is not to imply that research should be curtailed in this respect; it is simply stating that for some cases it may not be necessary to employ the most advanced hydrodynamic techniques for the analysis of certain water quality problems. On the other hand, the use of these techniques in analyzing the distribution of conservative substances and in some problems, e.g. simple single-stage nonconservative variables, is obviously appropriate. The success of this approach in such problems as the time and space distribution of salinity is noteworthy. However, with respect to the majority of the problems which involve nonconservative substances, the application of advanced hydrodynamic modeling techniques yields little additional information on the phenomena occurring because of the lack of knowledge of the complex water quality reactions. Until the gap in fundamental understanding between the two fields is narrowed, the excellent work of the hydrodynamicist, particularly over the past decade, is of value for only a limited number of estuarine quality problems. The majority of the water quality problems involving nonconservative substances with consecutive reactions, feedback, and higher-order life forms are only marginally improved in understanding by the use of advanced hydrodynamic modeling.

In summary, for conservative substances and single-stage non-conservative substances with simple reaction kinetics, water quality modeling in estuaries is well advanced for both spatial and temporal analysis. In this case, the problem is primarily a hydrodynamic one and this field is sufficiently developed to provide fundamentally realistic and useful models of water quality. On the other hand, systems that include non-conservative substances with a series of consecutive and feedback reactions are less well understood. Some modeling efforts have been initiated which appear to be fruitful. The complexities of most of these systems, however, outweigh the hydrodynamic effects and attention should be directed to the understanding and modeling of these phenomena in which the hydrodynamics play a minor role (in the sense of understanding the phenomena). Between the two extremes lie a variety of practical problems in water quality, in which both the reactions and transport may be equally significant. The extent to which each is important and therefore the type of model to use must be carefully assessed in each particular case.

It is therefore recommended that future research efforts be directed to an understanding and development of the reactions occurring in estuarine waters relating to physical, chemical and biological parameters. The latter two categories are particularly complex, because of the recycling and feedback mechanisms which produce pronounced nonlinearities in the equations. Support should be directed to the analytical development and solution of such models as well as field surveys to provide the necessary data for verification and evaluation.

More specifically, the following recommendations are offered with regard to future directions that should be taken on the modeling of estuarine water quality, and reflect a need to investigate model structures that are relevant to water quality management problems. The recommendations are not presented in any order of priority.

(1) Phytoplankton Models. Continual and expanded efforts should be devoted to the additional application of available approaches to areas of specific interest and to the development of new models which will adequately reflect interactions between several nutrient constituents, phytoplankton and zooplankton. The effect of seawater intrusion in estuaries and bays on the species composition and subsequent effects on the total phytoplankton population is one example of phenomena that are yet to be modeled.

(2) Dissolved Oxygen Models. Contrary to widely held opinions in the field, the dissolved oxygen phenomena in estuaries are not completely understood. This lack of understanding applies especially to the role that nitrogeneous discharges play in oxygen utilization, e.g. the "competitive" use of ammonia by algae and nitrifying bacteria. In addition, the use and generation of oxygen by phytoplankton and the subsequent use of oxygen by bacteria in oxidizing algal carbon still require analysis and mathematical model construction. There is an obvious interplay here between the phytoplankton models and the DO models.

(3) Nutrient Models. These models form a subset of models that generally must be solved together with models of phytoplankton growth and dissolved oxygen. Included here are various nitrogen and phosphorous forms, interactions and significant sources and sinks. Bottom sediment exchanges and seawater intrusion effects are particularly important.

(4) Models of Intermediate Levels of Food Chains. A variety of estuarine situations revolve about interactions between water quality, phytoplankton and higher levels of the food chain. There are virtually no models available which relate in a meaningful way the effects of waste discharges on intermediate levels of estuarine flora and fauna. A typical example in this regard is the lack of any quantitative model relating environmental conditions to the distribution of opossum shrimp (Neomysis awatschensis), an important representative of the intermediate level of the food chain in the San Joaquin Delta in California.

(5) Fishery Resource Models. There are significant water quality problems that interact directly with juvenile and adult fish populations. An example is the effect of dissolved oxygen levels on the passage of anadromous fish such as the American Shad. Verified models are required to describe the effects of waste reduction programs on the population dynamics of such populations. Included in these models should be the effect of regional fishing pressures, "natural" environmental variations (temperature, salinity, etc.), as well as the effects of time-variable waste discharges and river flows.

(6) Chemical Kinetic Models, Group I. The modeling of complex reaction kinetics in estuarine systems has rarely been attempted. The full nonlinear kinetic interactions superimposed on the transient buffering capacity of seawater represents an area of water quality modeling that can pose formidable conceptual, mathematical, and computational problems. In this first group, a need exists to model such variables as iron, manganese, and various sulfur forms all of which may play important roles (such as interactions with bottom sediments) in the total water quality distribution in estuaries.

(7) Chemical Kinetic Models, Group II. In this group, are included the acidic or alkaline discharges from concentrated industrial wastes. These types of discharges interact with the carbon dioxide system which is considered in this grouping. The CO_2 system also interacts with the phytoplankton models discussed in (1) above. Again, these chemical systems involve complex nonlinear equations, whose behavior is poorly understood. In addition, some of the chemical reactions accompanying the discharge of acids, alkalis or other wastes are associated with precipitates which may produce water use problems. The deposition of solids and particulate matter must therefore also be modeled in a workable, meaningful fashion (see also (9) below).

(8) Near-Shore Waste Disposal. There is a complete absence of any unified mathematical model approach toward describing the effect of a waste discharge in the near-shore environment (generally the continental shelf limits). The increasing tendency to utilize the oceanic environment for the disposal of municipal and industrial waste, sludge, toxic chemicals, dredge spoil, and solid wastes requires models of shelf circulation patterns, assimilation capacity in terms of organic material and nutrient enrichment. These models will require a close interaction with viable hydrodynamic circulation models and biological and chemical models. The problem context is generally multidimensional and will pose significant computational (and conceptual) problems.

(9) Particulate Matter Models. As indicated in (7) above, some discharges of waste into the estuarine or near-shore environment are accompanied by chemical precipitates, the distribution and settling patterns of which must be modeled. The settling characteristics of dredge spoil in the estuarine or shelf areas determine the ultimate bottom distribution of such spoil and hence the effects on bottom flora and fauna. As a final example, the zone of influence of ocean outfalls on bottom life due to the distribution of sewage or sludge solids must be modeled.

(10) Gas Transfer Models (Air-Sea Boundary Phenomena). Several of the variables indicated above, including oxygen, CO_2 and nitrogen all ultimately involve some type of gas transfer phenomena at the air-sea boundary. Submodels are necessary to relate these exchanges to such variables as wind speeds, wave conditions and salt content. Successful formulation of such models would provide an important input for the more macroscopic models discussed above.

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DISCUSSION

THOMANN: I think many of the points that have been raised already to some extent underly the philosophy of our approach. What we have done is to try to place an emphasis on summarizing some of the more important kinds of water quality problems. We proceed from general steady-state equations. These, to my mind, are still extremely valid approaches to many problems that we face in water pollution control which are of a longer term, capital-improvement, capital-intensive type problem. That is, people ask questions such as: if we want to improve our level of treatment to a certain degree, what do you think is going to happen over the long haul? So steady-state models still, I think, have a large part to play in water quality modeling. We proceed from one-dimensional analyses, from constant-area steady-state solutions (some one-dimensional analytical impulse-response solutions) into conservative substances and some non-conservative substances (we emphasize again the fact that the non-conservative nature of the system can be important), and then go into consecutive reactions, which form the basis, of course, for the classical BOD-DO type models.

We indicate here, in a very general way, the interaction between one species, in this case c_1 in Equation (3.21), and how that acts as a source into a second species, c_2 in Equation (3.22). That kind of interaction is then built upon in the following section on multistage consecutive reactions. The idea here is to try to display the interaction between different water quality variables without, at this stage anyway, introducing the complexity of time-variable phenomena or detailed types of dynamic considerations. Equation (3.26), for example, is an illustration of a four-stage consecutive reaction system in the context of nitrification, species N_1 being organic nitrogen, N_2 being ammonia nitrogen, N_3 being nitrite, and N_4 being nitrate. Again, here we just simply introduce the coupling between these equations as closeup simple first-order reaction kinetics.

The order of magnitude of those rate coefficients governs greatly how the system responds and to what extent the feedforward reactions occur. These equations have no feedback in them at all (and later on in this chapter we discuss some of the possibilities of introducing steady-state feedback). Essentially we know very little about these reaction coefficients. For the simply coupled system, BOD-dissolved oxygen type system, we have a fairly good idea of what is happening. We are not completely in the dark. We know at least some order of magnitude of the possible responses that may occur due to carbon sources, that is, oxidizable carbon being discharged, and the resulting dissolved oxygen deficits. In the case of nitrogen, the only place I've really seen any substantial work done in this area in the past has been in the Thames, where they attempted to measure some of the rates of ammonia oxidation. We have since done a fair amount of work on some modeling on the Delaware and the Potomac where we tried to pin down some of those reaction rates using available field data.

We have tried to place an emphasis on the kinds of interactive reaction kinetic systems that are of importance in describing water quality problems. I think I'd like to draw your attention to Equation (3.42), and subsequently Equations (3.43) and (3.44), to highlight the importance of these reaction kinetics. Equation (3.43) has a diagonal matrix introduced with a reaction term K_d , which is the classical deoxygenation rate. You see it's a multiplicator factor. It ends up multiplying everything that appears to the right-hand side of that. Now in those matrices $[A]^{-1}$ and $[B]^{-1}$ is a conglomeration of dispersion and advection effects, and that total matrix product that you see there responds most sensitively to those reaction kinetics. There is an illustration of where it certainly is of some importance.

Equations (3.43) and (3.44) display the kinds of systems that result from consecutive-type reactions without any feedback, nitrification being an example, shown in Figure 3.4. Now there's a four-system model, outputs of which are then fed into a dissolved oxygen model to track four different forms of nitrogen, and the utilization of oxygen in the oxidation of ammonia and nitrite. That is a fairly simple model of the nitrogen system at this stage. As I said, it incorporates no feedback loops, nor does it incorporate the fact that any of these nitrogen forms, especially the ammonia and the nitrate, are nutrient sources for phytoplankton growth. But as a sort of a framework for describing nitrification effects due to the discharge of large amounts of oxidizable nitrogen, it has proven to be useful in describing the effects on the dissolved oxygen deficit. And that, as has been pointed out, can be very, very substantial. The little circles there are the reaction coefficients. Those are the ones that are somewhat difficult to pin down and, we believe, really require a fair amount of additional work.

We also make the point that we don't believe that the state-of-the-art at this stage is up to rigorous statistical comparisons, generally, between output from some of these water quality models and observed data. More often than not, our observed data are somewhat limited, and there is undoubtedly at this stage an amount of judgment that is still rampant in our analysis of whether, in fact, we have a valid model.

RATTRAY: I guess I have one concern, and that's about making a simplified, one-dimensional hydrodynamic model and then putting in a whole bunch of time-dependent interactions, and saying, "Aha! Our limitation in predicting what happens is due to the lack of knowledge of reaction rates." And we've forgotten that that's the part that hasn't been simplified to have just one number. You forget the fact that you're talking about an oversimplified hydrodynamic model for many of the kinds of problems you might be concerned with. If you put in a two- or three-dimensional hydrodynamic model, then the final result might be quite dependent upon some of the parameters in that kind of a model. What would happen with an oil spill interacting with the upstream migration of a biological population which stayed in the lower layer? You could know the reaction rates perfectly, but if you didn't know how much the populations overlapped, you couldn't tell how they interacted. So there are cases where you have to know how much of the time these different kinds of concentrations are overlapping, and at what concentrations they are overlapping. I think we can't neglect the fact that some of the hydrodynamics will be important even though we need to know reaction rates, too. So this is just adding a little bit, I think, to what was said.

THOMANN: I think that that reinforces the point that when one runs into the kind of situation you just mentioned, one most obviously has to go to a more complicated hydrodynamic situation, taking cognizance of vertical or lateral gradients.

RATTRAY: Agreed.

THOMANN: I guess what we are responding to, again, is the general order of most of the water quality problems that seem to be in existence today. Oil spills, there is no question that it's a water quality problem. I don't know whether we've ever developed a state-of-the-art to deal with that kind of situation, since this was a state-of-the-art report. There are no models that we know of for dealing with oil spills.

HARLEMAN: Basically, the problem of the nonadvective tidal models, which is one of the problems which hasn't been brought up, is the longitudinal fogging which these introduce. That is, by in a sense ignoring the tidal motion you somehow automatically introduce a longitudinal fogginess which is of the order of magnitude of the tidal excursion, which is of the order of magnitude of five to ten miles in most estuaries. When we come down to talking about local problems, certainly this kind of fogginess is going to introduce difficulties. We get one thing if we talk about low water slack, and we get something else if we talk about high water slack. Again, when you come to the question of sampling, the problem of what you sample and how you sample must first be determined by, obviously, what kind of model you are going to use the data in. And in many ways a short period of sampling, fairly intense, is much more adaptable to the so-called real time models because you can deal with quantities taken over a relatively short time and hopefully make some sense out of it. But if you are going to use a freshwater advection model then you need to really do a lot more sampling because of this longitudinal fogginess, which is really in there. I think in some ways this has been largely overlooked. If you ignore the tidal motion then, really, how can you pin down quantities within a distance of a tidal excursion? And at the same time, I don't follow really Dr. Thomann's argument that when you are dealing with large reaction coefficients, that is, when things are pretty much controlled by large decay terms, that you can then dispense with worrying about the tidal motion, because it seems to me that then you need to be more concerned with real time behavior. Just think about time of travel. The particle of water is moving up and down the estuary very large distances every tidal period.

THOMANN: What I meant to imply is that with higher reaction rates the system is more sensitive to those reaction rates than it is to dispersion.

HARLEMAN: It is also sensitive to real time and not twelve-hour averages.

THOMANN: But all of our problems need not be solved on a real time basis, or what we are calling a real time basis. There are any number of problems with which we are confronted that are the kinds of seasonal-type phenomena that don't require that kind of time scaling. I think that's the point that we are getting at. In those kinds of seasonal, quasi-steady-state situations, we can turn that dispersion knob an awful lot in one direction or the other. For higher reactive systems it is not going to make a significant difference. That was the point.

PRITCHARD: Well, with regard to this discussion of being concerned with what happens in time and space over scales of the order of a tidal excursion or less, or whether or not we can be concerned with a grosser picture, again I've got to draw on my own experience in a system where quite frequently it depends on whether we are looking at close-in distributions or distributions well away from the source. If you happen to be in a small waterway where twelve miles is most of the waterway then you ought to be concerned with the tidal time everywhere. But if you're concerned with a large waterway, there you may only be interested in real time in a close space within a certain distance up and down from the outfall.

THOMANN: What we seem to be saying is that when the problem demands it, one goes to a small time and small space model. I think my point is that many of the problem contexts in which we find ourselves as far as pollution control is concerned are generally not of that type. They are generally more of the sort of longer term, capital intensive. If we do this generally to our waste load discharges in this area, what do we expect to have happen?

PRITCHARD: Well, I think that depends on where you are in the system decision. Maybe that's what FWQA has to consider overall, but not in a day-to-day response to an actual decision. For instance, in my case, does the state approve water use of this particular plant? I've got to know what it does locally as well as what it does on a large scale.

HARLEMAN: I still think there's a fallacy of assuming in going to more computation that this is only a question of whether it's warranted from the whole time span. I still maintain that by closing down on the time scale one gets a better computational scheme and less adjustable coefficients. Even if your interest extends over a year, it may well pay off in the end to spend more time on the computer to generate a lot more time data than you're really every going to use, because by doing this you avoid introducing arbitrary unknown coefficients which take up the thing that you haven't spent the time computing. It's not really a question of just deciding on the time span. It may well pay off to do it on a small time scale and spend more time on the computer and only use the results once a day that you get out.

THOMANN: Yes. I think, as you pointed out, that it's essentially the same. I still see it as a trade-off as to whether in fact it's worthwhile in any particular problem context to throw the computational time associated with the real time model into a dispersion coefficient, an over-a-tidal-cycle dispersion coefficient, on which the problem solution doesn't depend to a large extent anyway. That's the point. It's not completely dependent on that coefficient. And it may very well prove worthwhile to make that trade-off.

I think part of the problem revolves around how one looks at the time scales that are of importance. If there is a local, within-tidal time phenomenon, as just pointed out, then, obviously, yes. There are a number of problems, however, where seasonal effects, yearly effects, and we might be concerned with running these models for periods of ten, fifteen or twenty years. Then working on an hourly time frame, it seems to me, would not be the way to go. Suppose I want to estimate the effects over a fifteen or twenty year flow hydrograph of ways to control, and what I expect to happen to the water quality. Then would we do that on an hourly time step? Probably not. At least I don't think so.

PRITCHARD: Well, if the dynamics required it, I think you'd have to.

THOMANN: Well, the point there is that the time gradients, in a sense, of the seasonal fluctuations and weekly fluctuations, are probably orders of magnitude greater than what's happening over a tidal cycle. For example, take dissolved oxygen, which fluctuates from fourteen, twelve, thirteen mg/l down to zero. Over a year you don't get those kinds of time fluctuations over a tidal cycle.

WASTLER: Well, you could get a fair percentage of them over a tidal cycle.

THOMANN: Only if you advect from complete saturation and go right past a zero DO location. That would be the only way, and that would be an extremely sharp spatial gradient.

PRITCHARD: There are a lot of regions, eutrophic regions, where you have die-off at night and the DO goes from supersaturation to pretty low values overnight.

THOMANN: In which case one runs that kind of model.

PRITCHARD: Yes. Agreed.

RATTRAY: We've got to worry a little bit about differentiating space scales and time scales. Tidal motion has not only different time scales, but space scales. In some cases the problem is the fact that they are different space scales and in others it's time scales.

DOBBINS: The things that need more work than anything else are the mechanisms, the assimilation of the various types of inputs. We don't know enough about these inputs, the interrelationships between these inputs, and I think, if we are going to use these things for predictive purposes, it is very important that we clarify some of these processes. These linear equations assume that if we take the individual effect of any particular input and we remove that input from the system then its effect will be removed. The only trouble is nature doesn't necessarily act that way. And when we remove some inputs, we change the ecological system and make it trigger new inputs. A very crude example. If you take the silt out of a polluted river, the water doesn't turn clear. It turns green. These are problems for which we need some answers before long, if we are going to avoid spending billions of dollars and finding out that we're not accomplishing what we hoped to accomplish. The City of New York, for example, has under design treatment plants that will cost over a billion dollars to build. A very serious question in my mind is whether or not this expenditure is going to make the changes some people are currently anticipating. It's a very, very serious question.

And so we are interested in the water quality and not just the hydrodynamics of these systems. The assimilation mechanisms.

PRITCHARD: It seems to me that we are a lot further ahead in the physics than we are in the biology.

DOBBINS: That's right.

PAULIK: As a biologist, I'm happy to see engineers at least recognize the problem. This should receive high priority in the future. We should begin to look at the sources and sinks, and the non-conservative properties of the system.

DOBBINS: It's not so much a question about the reaction rates; we don't even know what reactions take place. The type of cycles. We can't even draw diagrams.

THOMANN: Well, we're not completely ignorant. It's just that we're not nearly as sharp as we are in the hydrodynamic area. I think there is an order of magnitude of difference between the level of understanding there and in the water quality.

CHAPTER IV

ESTUARINE TEMPERATURE DISTRIBUTIONS

John Eric Edinger

1. NATURAL TEMPERATURE DISTRIBUTIONS

Water temperature observations are an integral part of almost every type of estuarine study. Gas and salt solubility, biological and chemical reaction rates, and density and viscosity are all functions of water temperature. Water temperature has been an ancillary variable. Despite the wealth of data that might be available, a systematic description of the spatial and temporal distribution of temperature has not, until recently, been an important part of estuarine hydrography.

Salinity dominates the density structure of an estuary. The density difference due to a gradient of 1 o/oo of salinity is about equal to that produced by a 7°F temperature differential. In the formulation of large-scale estuarine circulation, the density and buoyancy terms in the equations of motion are adequately described by relation to the salt concentration and its conservation expression. It has not been necessary, fortunately, to develop the heat budget and consequently the spatial and temporal temperature distribution for inclusion in the momentum balance of an estuary. The influence of temperature on density structure becomes important locally, in the vicinity of advective heat sources such as steam electric power plant condenser cooling water discharges and in the description of buoyant convection near the water surface particularly as related to surface heat exchange.

Circulation and mixing within an estuary are described and classified by the salinity distribution resulting from the interaction of a freshwater inflow at the head of the estuary and a high salinity source at the ocean end (Pritchard 1955). This description is related to the dominant advective and dispersive terms in the salt conservation equation. A classification of estuarine temperature distributions can be developed within the classification scheme of estuaries based on salinity by assuming that the advective and dispersive processes that are dominant in the salt conservation equation for a particular estuary are also dominant in the heat conservation relation describing the temperature distribution. In addition to the dominant advective and dispersive processes, it is necessary to include surface heat exchange and attenuation of short-wave radiation with depth in the heat conservation equation.

1.1 SIMILARITY BETWEEN SALINITY AND TEMPERATURE DISTRIBUTIONS

When surface heat exchange and artificial heat sources are a small fraction of the estuarine heat budget, the temperature distribution, like the salinity distribution, is controlled by the temperature of the freshwater inflow at the head of the estuary and conditions at the ocean end. Salinity is generally higher at the ocean end of the estuary than at the freshwater end, but temperature can be higher at the freshwater end than at the ocean end, as during a summertime condition, or lower at the freshwater end than at the ocean end, as during a wintertime condition. When the freshwater inflow temperature is less than the ocean temperature, the temperature will increase from the head of the estuary to the mouth and increase from the surface downward as does salinity. When the freshwater inflow temperature is greater than the ocean temperature, temperature will decrease from the head of the estuary to the mouth and decrease from the surface downward.

The similarity between the salinity distribution and temperature distribution can be expressed in terms of a temperature differential where the base temperature is taken as the freshwater inflow temperature T_r such that zero temperature differential corresponds to zero salinity. The ocean salinity S_o would correspond to the maximum temperature differential, which is $T_o - T_r$ where T_o is the ocean temperature. The relationship between the temperature $T(x,y,z)$ and the salinity $S(x,y,z)$ for any point in the estuary can be stated at least as a proportionality as

$$\left[T(x,y,z) - T_r\right] / \left[T_o - T_r\right] \sim S(x,y,z)/S_o \tag{4.1}$$

which applies to either condition of the freshwater inflow temperature being greater or less than the ocean temperature. This similarity relation is stated for steady-state conditions because the freshwater inflow temperature T_r will vary independent of the circulation within the estuary. Simultaneous temperature and salinity distributions presented by Owen (1969) and reproduced here in Figures 4.1 and 4.2 qualitatively demonstrate the similarity relation. Figure 4.1 shows a wintertime condition with $T_r < T_o$ and Figure 4.2 shows a summertime condition with $T_r > T_o$.

Any difference between an observed temperature distribution and a temperature distribution determined by similarity to salinity should be attributable to surface heat exchange, attenuation of short-wave radiation, groundwater inflow and advective sources other than freshwater inflow. Similarity between salt and conservative temperature distributions may also differ if the diffusivities for salt are not the same as for heat.

1.2 INFLUENCE OF SURFACE HEAT EXCHANGE ON TEMPERATURE DISTRIBUTIONS

The freshwater inflow and ocean water mixed to the surface layers of an estuary are heated or cooled by exchange of heat across the water surface. Inclusion of surface heat exchange in the description of estuarine temperature distributions complicates in particular the longitudinal distribution of surface temperature and, consequently, the vertical temperature distribution.

Heat is exchanged across the water surface by shortwave solar and longwave atmospheric radiation $H_s + H_a$, radiation reflection $H_{sr} + H_{ar}$, longwave back radiation H_{br}, evaporation H_e, and conduction H_c. The net rate of surface heat exchange H_n is defined as

$$H_n = (H_s + H_a - H_{sr} - H_{ar}) - (H_{br} + H_e + H_c) \tag{4.2}$$

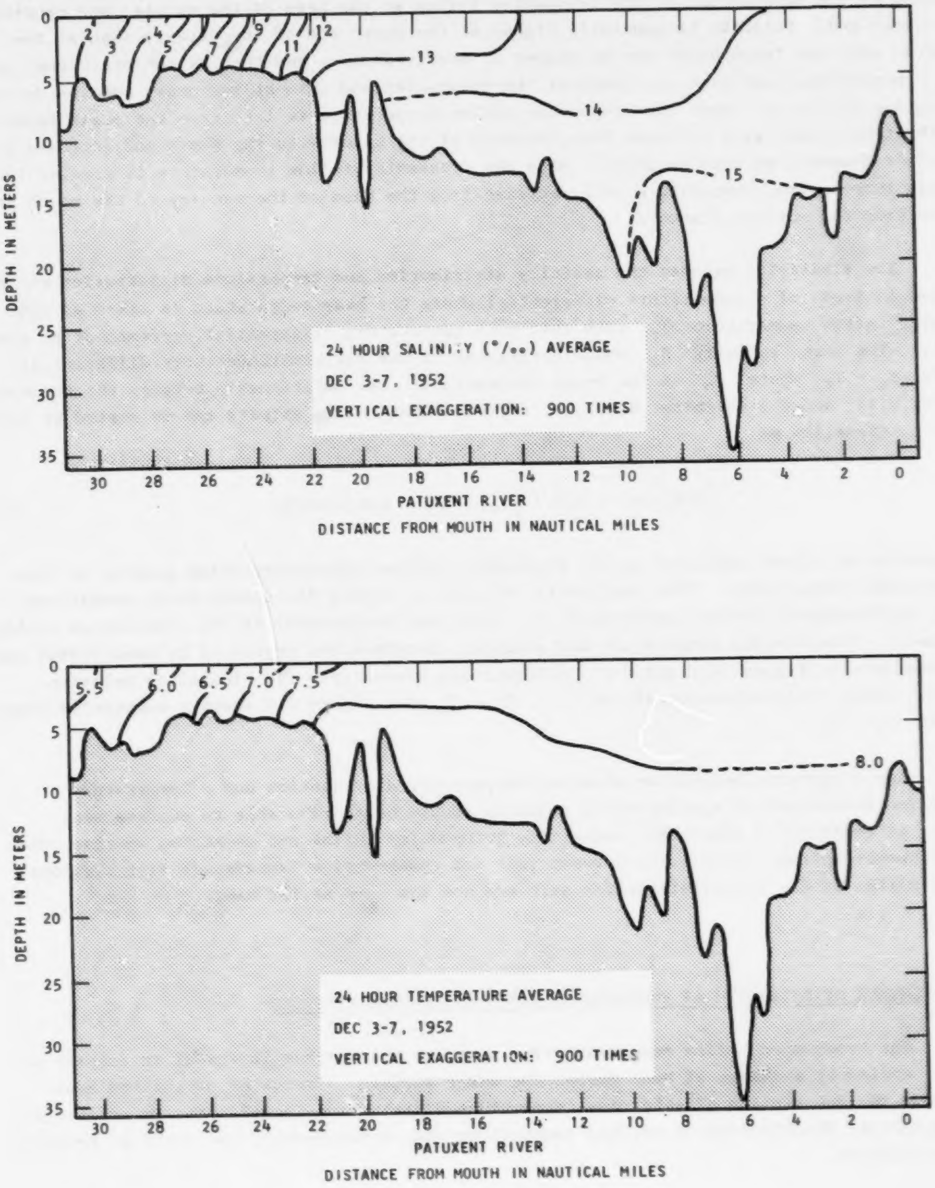


Fig. 4.1 Mean Salinity and Temperature in Patuxent Estuary: Winter. From Owen (1969).

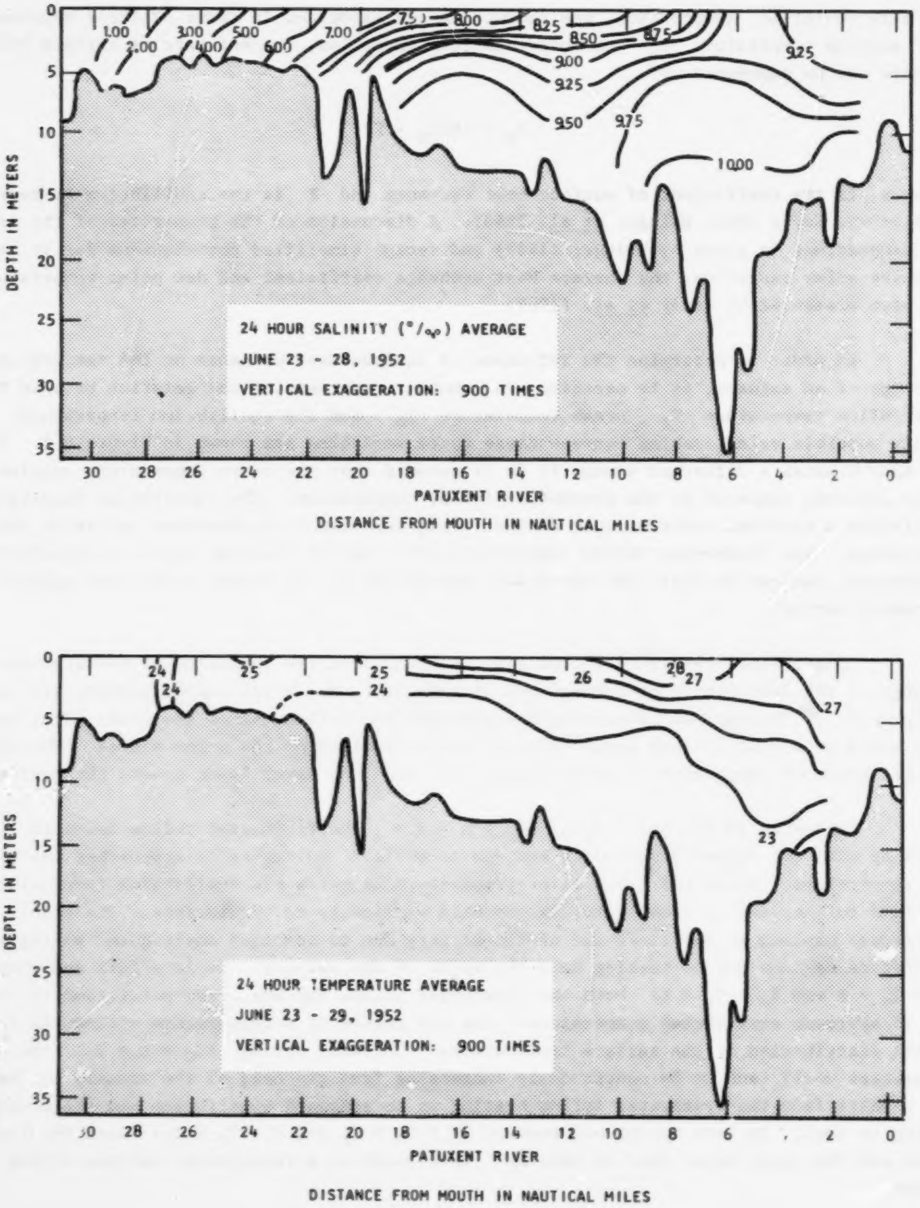


Fig. 4.2 Mean Salinity and Temperature in Patuxent Estuary: Summer. From Owen (1969).

When back radiation, evaporation, and conduction are expressed in terms of their dependency on water surface temperature T_s and meteorological variables, the net rate of surface heat exchange can be expressed as

$$H_n = -K(T_s - E) \tag{4.3}$$

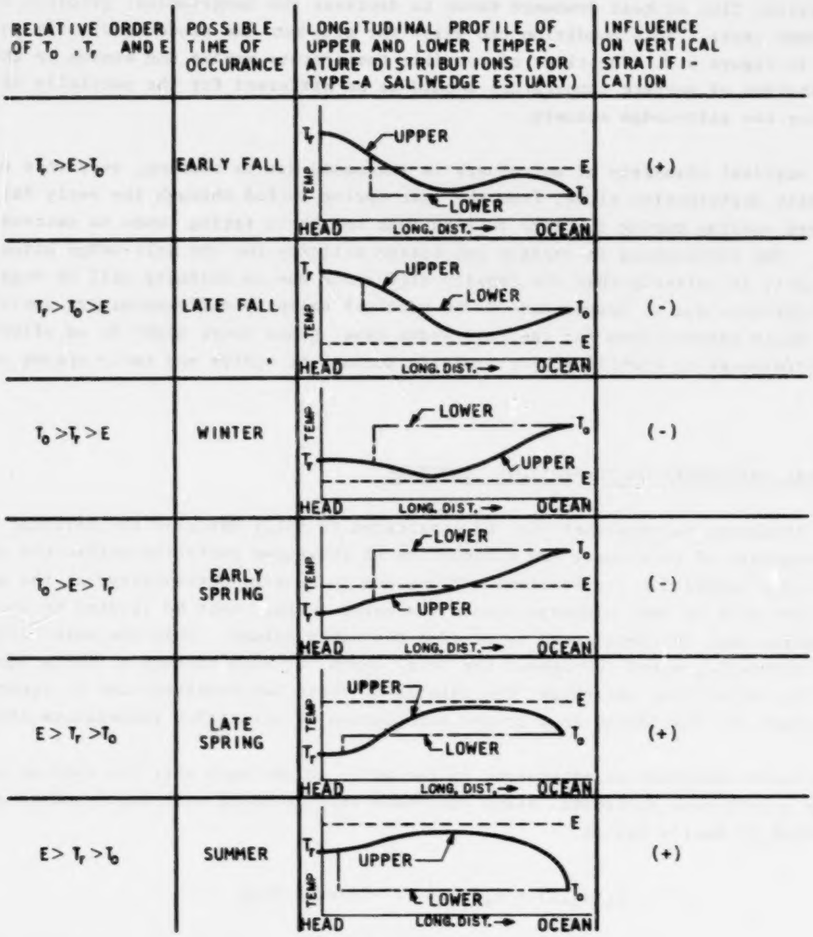
where K is the coefficient of surface heat exchange and E is the equilibrium temperature (Edinger and Geyer 1965, Edinger et al. 1968). A discussion of the properties of the equilibrium temperature is given by Edinger (1969) and recent simplified formulations for it based on shortwave solar radiation, the surface heat exchange coefficient and dew point temperature have been presented by Brady et al. (1969).

In order to determine the influence of surface heat exchange on the temperature structure of an estuary, it is necessary to consider each case of the relation between freshwater inflow temperature T_r, ocean temperature T_o, and the equilibrium temperature E. The six possible relationships between these three variables are shown in Figure 4.3. Each case approximates a different season if it is assumed that the ocean temperature remains relatively constant compared to the freshwater inflow temperature. The equilibrium temperature will follow a seasonal cycle because of the strong dependency on shortwave radiation and air temperature. The freshwater inflow temperature will lag the seasonal cycle of equilibrium temperature, and can be less than the ocean temperature in the winter period and greater in the summer period.

Longitudinal temperature profiles resulting from the inclusion of surface heat exchange in the description of temperature distributions for a salt-wedge estuary are shown in Figure 4.3. The salt-wedge case is the simplest to consider since the lower layer temperatures would be almost uniform longitudinally and determined by the ocean source. The dominant vertical transport mechanism is an advective flux from the lower layer toward the surface.

Beginning in the early fall $(T_r > E > T_o)$, the freshwater inflow tends to cool due to mixing with the colder ocean water and due to surface cooling as it approaches the equilibrium temperature. Since the lower layer temperature is below the equilibrium temperature it will tend to increase as ocean water is advected vertically to the surface. The result is a temperature minimum at the river end of the estuary due to combined cooling and mixing and a temperature maximum due to heating near the mouth of the estuary. In late fall and winter $(T_r > T_o > E$ and $T_o > T_r > E)$ both the freshwater inflow and the ocean water tend to cool and tend to approach equilibrium temperature. The net result is a temperature minimum in the longitudinal distribution of the surface temperatures. In early spring $(T_o > E > T_r)$ the surface temperature would tend to be continuously increasing from the head of the estuary to the mouth. This results from the freshwater inflow heating up to approach equilibrium and the ocean water tending to cool. In late spring and summer $(E > T_o > T_r$ and $E > T_r > T_o)$ both the freshwater inflow and the ocean water tend to warm up. This leads to a temperature maximum within the estuary.

The partially mixed estuary is characterized by a longitudinal gradient of salinity in the lower layer. This is due to vertical flux from the lower layer to the upper layer by a combination of vertical advection and turbulent exchange of salt. The lower-layer temperatures decrease from the mouth of the estuary to the head of the estuary when $T_r < T_o$ and increase from the mouth to the head when $T_r > T_o$. When the lower layer is warmer than the surface layer there is a vertical turbulent flux of heat upward in the same direction as the turbulent



RELATIVE ORDER OF T_o, T_r AND E	POSSIBLE TIME OF OCCURANCE	LONGITUDINAL PROFILE OF UPPER AND LOWER TEMPERATURE DISTRIBUTIONS (FOR TYPE-A SALTWEDGE ESTUARY)	INFLUENCE ON VERTICAL STRATIFICATION
$T_r > E > T_o$	EARLY FALL		(+)
$T_r > T_o > E$	LATE FALL		(-)
$T_o > T_r > E$	WINTER		(-)
$T_o > E > T_r$	EARLY SPRING		(-)
$E > T_r > T_o$	LATE SPRING		(+)
$E > T_r > T_o$	SUMMER		(+)

Fig. 4.3 Tendency of Estuarine Upper and Lower Temperature Distributions When Influenced By Freshwater Inflow Temperature (T_r); Ocean Temperature (T_o); and Equilibrium Temperature of Surface Heat Exchange (E).

salt flux. This condition exists when $T_o > T_r$ or for the winter to late spring sequence of Figure 4.3. The tendency is for less heat to be transported vertically near the head of the estuary than at the mouth, hence the river end of the estuary responds more to the equilibrium temperature (i.e., surface heat exchange) than to the ocean temperature.

When the surface layers are warmer than the bottom layers in the partially mixed estuary the turbulent vertical flux of heat is downward and opposite to the vertical flux of salt. The vertical flux of heat downward tends to decrease the longitudinal gradient of temperature in the lower layer. This condition can exist for all but the winter and early spring periods shown in Figure 4.3. The times of possible temperature maxima and minima in the longitudinal distribution of surface temperature should be no different for the partially mixed estuary than for the salt-wedge estuary.

The vertical stability of an estuary is increased due to heating, over that resulting from the salinity distribution alone, from the late spring period through the early fall period. The trend toward cooling during the late fall through the early spring tends to decrease vertical stability. The differences in surface and bottom salinity for the salt-wedge estuary are quite large and it is unlikely that the density difference due to salinity will be negated by the density difference due to temperature. The vertical salinity differences are smaller for the partially mixed estuary than for the salt-wedge case, hence there might be an effect of temperature differences on stability, particularly during the winter and early spring periods.

1.3 ADDITIONAL INFLUENCES ON TEMPERATURE STRUCTURE

Two important factors that must be considered to fully describe the vertical temperature structure of an estuary are attenuation of shortwave radiation within the water column and buoyant convection (or vertical motions due to density instability) at the water surface. The net rate of heat exchange across the water surface must be related to the processes by which heat is transferred up or down the water column. When the water column can be considered vertically mixed throughout the total depth, or even through a finite identifiable depth in a stratified waterbody, the details of these two processes can be ignored. They must, however, be considered in a proper formulation of stratified temperature structure.

Shortwave radiation is attenuated in the water column such that the rate at which it passes through a unit-area horizontal plane decreases exponentially with depth and is described by a modification of Beer's Law as

$$H_s(x_3,t) = H_s(t) \cdot (1 - \beta)\exp(-\alpha x_3) \qquad (4.4)$$

where $H_s(t)$ is the rate at which the net shortwave radiation crosses the water surface and is a function of time depending on the angle of the sun and cloud cover, α is the attenuation coefficient and is a function of turbidity and chemistry of the water, $H_s(x_3,t)$ is the rate at which shortwave radiation passes a plane at depth x_3, and β is the fraction of $H_s(t)$ immediately absorbed at the surface (Dake and Harleman 1969). The rate of heat absorption due to shortwave radiation attenuation in a unit volume of fluid at depth x_3 below the water surface is

$$h(x_3,t) = -\frac{\partial}{\partial x_3} H_s(x_3,t) = H_s(t) \cdot \alpha \cdot (1 - \beta)\cdot\exp(-\alpha x_3) \qquad (4.5)$$

Normally in an estuary the attenuation coefficient α is thought to be so large that most of the shortwave radiation is absorbed near the surface. However, if α is small and if the estuary is sharply stratified, as for example a salt-wedge estuary, only a small portion of the shortwave radiation absorbed in the deeper layers is transported back to the surface. The lighter surface layer can create a greenhouse effect which results in a very high temperature in the lower layer relative to the surface temperature during the winter months.

In order to relate surface heat exchange to a continuously varying vertical temperature structure it is necessary to have a boundary condition at the surface accounting for the vertical heat flux into the water column. The necessary condition can be stated as

$$H_n - (1 - \beta)H_s(t) = \rho c_p K_3 \frac{\partial T}{\partial x_3} \bigg|_{x_3=0} - b_c \tag{4.6}$$

where $H_n - (1 - \beta)H_s(t)$ is the difference between the net rate of heat exchange at the water surface and shortwave radiation absorbed within the remaining water column, and represents the amount of heat that must be transported away from or to the water surface by vertical dispersion and by a vertical heat flux b_c due to buoyant convection. If buoyant convection at the surface is ignored in computations of vertical temperature structure accounting for surface heat exchange, then very steep surface temperature gradients would be produced when $H_n > H_s(t)$. For the condition that $H_n < H_s(t)$ there would exist a positive temperature gradient at the surface (i.e., the temperature would increase with depth below the water surface). Evaporation at the water surface tends to increase the surface salt concentration, hence surface density, and takes place during either net heat gain or net heat loss across the water surface. Phillips (1966) details possible directions toward a description of the buoyant convection process at the water surface and indicates that formulation of the problem is far from complete.

Dake and Harleman (1969) have formulated the vertical temperature structure for fresh water resulting from surface heat exchange, attenuation of shortwave radiation, vertical dispersion and vertical convection. The convective process is accounted for by introducing a computational procedure that amounts to an internal heat balance through a finite depth below the water surface. The procedure requires that just enough heat be brought up to the surface for the temperature at one depth to always be equal to or greater than the temperature at a lower depth.

2. ANALYTIC DESCRIPTION OF ESTUARINE TEMPERATURE STRUCTURE

Derivation of a three-dimensional time-varying heat balance per unit volume of fluid produces a continuity relation which is identical to the salt balance in the storage, advection, and dispersion terms. An additional source term must be included to account for radiation attenuation below the water surface and to indicate that heat is generally non-conservative relative to the advection and dispersion processes. The differential expression for temperature distribution thus is

$$\rho c_p \left\{ \frac{\partial T}{\partial t} + u_1 \frac{\partial T}{\partial x_1} + u_2 \frac{\partial T}{\partial x_2} + u_3 \frac{\partial T}{\partial x_3} - \frac{\partial}{\partial x_1} K_1 \frac{\partial T}{\partial x_1} - \frac{\partial}{\partial x_2} K_2 \frac{\partial T}{\partial x_2} - \frac{\partial}{\partial x_3} K_3 \frac{\partial T}{\partial x_3} \right\} = h_p(x_1,x_2,x_3,t) \tag{4.7}$$

where T is the temperature at point x_1,x_2,x_3 and time t ; u_1 , u_2 , and u_3 are the velocity components; K_1 , K_2 , and K_3 the eddy coefficients for heat which may differ from those for salt; ρ and c_p are the specific weight and heat of the fluid; and $h_p(x_1,x_2,x_3,t)$ is the internal source or sink term. Spatial averaging and application of the concept of homogeneity can be applied to the heat balance in the same manner as for a salt balance.

The problem of including heat as a non-conservative property in estuarine models is one of relating the waterbody temperature structure to surface temperature, hence to surface heat exchange. Three models of progressively increasing complexity in vertical structure are chosen here to illustrate how they might be adapted as temperature models. First is the vertically homogeneous and sectionally homogeneous temperature distributions as adapted from the similar salt models of Pritchard (1958). Second is the two-layered segmented model (Pritchard 1967). Third are models that might be used to describe a continuously varying structure such as developed by Hansen and Rattray (1965).

2.1 THE VERTICALLY MIXED CASE

The assumption of vertical homogeneity leads directly to an expression relating internal temperature structure to water surface temperature. Thus at a point (x_1,x_2) in the surface coordinate plane, the vertically homogeneous heat balance can be written as

$$\frac{\partial}{\partial t}(hT) + \frac{\partial}{\partial x_1}(u_1 hT) + \frac{\partial}{\partial x_2}(u_2 hT) - \frac{\partial}{\partial x_1}\left(hK_1 \frac{\partial T}{\partial x_1}\right) - \frac{\partial}{\partial x_2}\left(hK_2 \frac{\partial T}{\partial x_2}\right) = - \frac{K(T-E)}{\rho c_p} \tag{4.8}$$

where u_1 and u_2 are the vertically homogeneous longitudinal and lateral velocity components and K_1 and K_2 are the vertically homogeneous longitudinal and lateral dispersion coefficients. The term $K(T-E)$ is the net rate of surface heat exchange where K is the coefficient of surface heat exchange, E is the equilibrium temperature, and T is the surface temperature which is the same as the temperature described in the storage, advection and dispersion terms. As for the vertically homogeneous salt distribution, given the velocity components and diffusivities, and necessary boundary and initial conditions, Equation (4.8) can be used to determine a temperature distribution. It should not be implied, however, that an estuary in which the salt distribution is adequately described by a vertically homogeneous relation will also have a vertically homogeneous non-conservative temperature distribution.

The sectionally homogeneous description also provides a direct relation between internal temperature structure and water surface temperature. The time-varying longitudinal temperature distribution for the sectionally homogeneous case including surface heat exchange can be written as

$$\rho c_p \left\{ \frac{\partial}{\partial t}(\sigma_1 T) + \frac{\partial}{\partial x_1}(\sigma_1 u_1 T) - \frac{\partial}{\partial x_1}\sigma_1 K_1 \frac{\partial T}{\partial x_1} \right\} = -w(x_1,t) \cdot K(T-E) \tag{4.9}$$

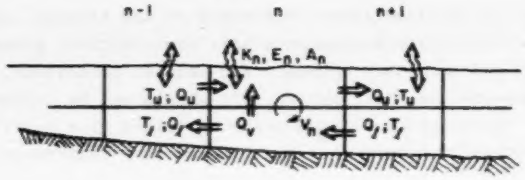
where the surface heat exchange term includes the surface width of the estuary $w(x_1,t)$ as a function of longitudinal distance and time. The coefficient of surface heat exchange K and the equilibrium temperature E are both functions of time and distance along the estuary. The longitudinal temperature profile $T(x_1,t)$ for the sectionally homogeneous case is determined by integration of Equation (4.9) after specification of the geometry, $\sigma_1(x_1,t)$ and $w(x_1,t)$; the sectionally homogeneous velocity $u_1(x_1,t)$; and a description of the longitudinal dispersion coefficient, the coefficient of surface heat exchange, and the equilibrium temperature. The boundary conditions are $T = T_r(t)$ at the head of the estuary and $T = T_o(t)$ at the mouth of the estuary, and correspond to the boundary conditions required for the sectionally homogeneous salt distribution. The steady-state solution of Equation (4.9) yields longitudinal temperature profiles whose shape depends on the order of T_o, T_r , and E , and takes the various forms given by the surface temperature distributions in Figure 4.3 with the exception that there would be no possibility of a temperature minimum for the early fall condition $(T_r > E > T_o)$.

The surface heat exchange condition of the vertically and sectionally homogeneous cases also holds for the segmented form of these vertically mixed models.

2.2 TWO-LAYERED SEGMENTED MODELS

Incorporation of surface heat exchange in a two-layered segmented model as used by Pritchard (1967) is possible if it is assumed that the heat transfer process of back radiation, conduction, and evaporation are a function of the upper layer segment temperature. The salt balance is extended to a heat balance by adding to the relationships of the upper layer the terms for surface heat exchange. Following the notation of Pritchard (1967), shown here in Figure 4.4, the steady-state heat balance for the upper-layer n th segment is

$$\begin{aligned}(Q_u)_{n-1,n}\left\{\frac{(T_u)_{n-1}+(T_u)_n}{2}\right\} + (Q_v)_n\left\{\frac{(T_u)_n+(T_\ell)_n}{2}\right\} + V_n\left\{(T_\ell)_n-(T_u)_n\right\} \\ = (Q_u)_{n,n+1}\left\{\frac{(T_u)_n+(T_u)_{n+1}}{2}\right\} + \frac{A_n \cdot K_n}{\rho c_p}\left\{(T_u)_n-E_n\right\}\end{aligned} \tag{4.10}$$



$(Q_u)_{n-1,n}$ = VOLUME RATE OF NET FLOW FROM THE (n-1) SEGMENT TO THE nth SEGMENT, UPPER LAYER.

$(Q_u)_{n,n+1}$ = VOLUME RATE OF NET FLOW FROM THE nth SEGMENT TO THE (n+1) SEGMENT, UPPER LAYER.

$(Q_\ell)_{n+1,n}$ = VOLUME RATE OF NET FLOW FROM THE (n+1) SEGMENT TO THE nth SEGMENT, LOWER LAYER.

$(Q_v)_n$ = VOLUME RATE OF NET VERTICAL FLOW FROM THE LOWER LAYER TO THE UPPER LAYER, nth SEGMENT.

V_n = VERTICAL EXCHANGE COEFFICIENT, nth SEGMENT.

$(T_u)_n$ = TEMPERATURE OF UPPER LAYER, nth SEGMENT.

$(T_\ell)_n$ = TEMPERATURE OF LOWER LAYER, nth SEGMENT.

E_n = EQUILIBRIUM TEMPERATURE AT nth SEGMENT.

K_n = COEFFICIENT OF SURFACE HEAT EXCHANGE AT nth SEGMENT.

A_n = SURFACE AREA OF nth SEGMENT.

Fig. 4.4 Notation For Two-Layered Segmented Temperature Model. After Pritchard (1967).

and for the lower-layer n th segment the heat balance is

$$(Q_\ell)_{n+1,n}\left\{\frac{(T_\ell)_{n+1}+(T_\ell)_n}{2}\right\} = (Q_\ell)_{n,n-1}\left\{\frac{(T_\ell)_n+(T_\ell)_{n-1}}{2}\right\} + (Q_v)_n\left\{\frac{(T_\ell)_n+(T_u)_n}{2}\right\} + V_n\left\{(T_\ell)_n-(T_u)_n\right\} \tag{4.11}$$

Rearranging the upper-layer segmented heat balance in such a form that the segmented temperatures are separated as linear variables gives

$$(T_u)_{n-1}\cdot(Q_u)_{n-1,n} - 2(T_u)_n\left\{V + \frac{K_nA_n}{\rho c_p}\right\} + (T_\ell)_n\left\{2V_n + (Q_v)_n\right\} = (T_u)_{n+1}\ (Q_u)_{n,n+1} + \frac{A_nK_nE_n}{\rho c_p} \tag{4.12}$$

Conceptually, the advection terms $(Q_u)_{n-1,n}$, $(Q_u)_{n,n+1}$ and $(Q_v)_n$ can be determined from the salt distribution and then utilized in the temperature equations. Specification of the boundary temperatures at the head and ocean end of the estuary, along with Equations (4.10) and (4.11) gives $2n + 2$ equations from which to determine the same number of unknown segmented temperatures. The vertical mixing coefficient V_n can be changed for heat from that found for salt.

One feature of the two-layered segmented salt balance is that it requires no specification of the segment geometry, although it does require judicious selection of the salinity values that apply at the segment boundaries when evaluating the advection terms. Extension to a temperature model requires specification of the surface area of the upper layer segments.

The influence of surface heat exchange on the two-layered temperature structure can be determined by comparison of the term $K_n A_n/\rho c_p$ numerically with V_n and with either $(Q_u)_{n-1,n}$ or $(Q_u)_{n,n+1}$ in Equation (4.12). If $K_n A_n/\rho c_p$ is small in comparison with both of these terms then the temperature distribution is controlled by the end conditions, as is salinity, and the similarity relation between temperature and salinity can be employed. The lower n th segment heat balance, Equation (4.11), can be extended by including a term for absorption of shortwave radiation, and the vertical advection term $(Q_v)_n$ may require modification to account for buoyant convection.

2.3 CONTINUOUS VERTICAL TEMPERATURE STRUCTURE

In each of the cases discussed above, the surface temperature could be explicitly related to a temperature in the advective and dispersive terms. This is not possible in cases where the temperature structure varies continuously through the vertical.

Relating the source term h_p in Equation (4.7) to the rate of heat absorption due to attenuation of shortwave radiation, Equation (4.5), gives the heat balance for a volume element below the water surface $(x_3 > 0)$. Integrating Equation (4.7) over the depth of the water column $h(x_1,x_2,t)$ and utilizing Equation (4.6), where the buoyant convection term b_c is related to the vertical advective flux at the water surface gives

$$\rho c_p \int_0^{h(x_1,x_2,t)} \left\{ \frac{\partial T}{\partial t} + u_1 \frac{\partial T}{\partial x_1} + u_2 \frac{\partial T}{\partial x_2} - \frac{\partial}{\partial x_1}\left(K_1 \frac{\partial T}{\partial x_1}\right) - \frac{\partial}{\partial x_2}\left(K_2 \frac{\partial T}{\partial x_2}\right) \right\} dx_3 = -K(T_s - E) \qquad (4.13)$$

where T_s is the surface temperature. Equation (4.13) is the most general heat budget that can be written relating the vertical temperature structure to surface heat exchange and attenuation of shortwave radiation below the water surface. Applying the concept of vertical homogeneity to Equation (4.13) reduces it to Equation (4.8).

The integral condition of Equation (4.13) requires knowing the internal temperature structure for its application; yet it must be satisfied to determine the temperature structure. At the same time the temperature gradient below the water surface must satisfy the buoyant flux relation of Equation (4.6), and attenuation of shortwave radiation, Equation (4.7). This suggests that determination of a continuously varying vertical temperature structure which is strongly related to surface heat exchange will require an iterative computation.

The iterative computations required to determine the internal heat balance of an estuary can be initiated from a conservative temperature distribution based on similarity to the salt distribution. Vertical salinity structure as predicted, for example, by the relationships developed by Hansen and Rattray (1965) would provide an initial temperature distribution. Relaxation of the conservative temperature distribution to satisfy Equation (4.13) could proceed using an empirical computation scheme similar to that of Dake and Harleman (1969).

It is obvious that the temperature structure of an estuary can be predicted in no more detail than the salinity structure. Further, the detail with which the vertical temperature structure can be predicted in an estuary is clearly limited by the ability to account for buoyant convection near the free water surface.

3. MODELING TEMPERATURE DISTRIBUTIONS DUE TO LARGE HEAT SOURCES

The modeling of the effects of large heat sources may be conveniently classified according to three spatial scales. First is the localized region in the immediate vicinity of the discharge and intake structures, which encompasses on the order of hundreds to thousands of feet. The temperature distribution in this region is principally controlled by the discharge configuration which can assume many forms depending upon the design constraints and the desired effects. The second scale for heated discharges could be named the intermediate region or transition region. This is the region in which currents and eddies within the receiving waterbody mix the heat from the localized region of the discharge to where its distribution is governed by the larger scale circulation, and typically extends over thousands of feet to tens of thousands of feet. The third scale considers the influence of the heat source on the large-scale temperature distributions, as discussed in Sections 1 and 2.

The present (1970) semiempirical basis for analytically describing the temperature distributions in each of these three regions is discussed. It is necessary to first introduce the concept of temperature excess as developed from the heat conservation relations. Also, a brief discussion of the application of physical hydraulic models to the study of large thermal sources is given.

3.1 THE TEMPERATURE EXCESS

The temperature excess can be defined for a single heat discharge as the difference between the temperature distribution with the discharge and the temperature distribution without the discharge (Pritchard and Carter 1965). This definition is made more precise from an analysis of the general heat conservation relation, Equation (4.7). Let $T(x_1,x_2,x_3,t)$ be the temperature related to the internal heat source term $h_p(x_1,x_2,x_3,t)$ and a given set of boundary and initial conditions. An additional heat source will result in a new total internal source of $h_p'(x_1,x_2,x_3,t)$ and temperature $T'(x_1,x_2,x_3,t)$. The temperature excess is then defined as

$$\theta(x_i,t) = T'(x_i,t) - T(x_i,t) \qquad (4.14)$$

Equation (4.7) would hold for $T'(x_i,t)$ as well as for $T(x_i,t)$ by inclusion of the additional heat source, as long as the velocity field $u_i(x_j,t)$ and the dispersion coefficients $K_i(x_j,t)$ remain unchanged. Then the expression for the conservation of excess temperature becomes

$$\rho c_p\left[\frac{\partial\theta}{\partial t} + u_1\frac{\partial\theta}{\partial x_1} + u_2\frac{\partial\theta}{\partial x_2} + u_3\frac{\partial\theta}{\partial x_3} - \frac{\partial}{\partial x_1}\left(K_1\frac{\partial\theta}{\partial x_1}\right) - \frac{\partial}{\partial x_2}\left(K_2\frac{\partial\theta}{\partial x_2}\right) - \frac{\partial}{\partial x_3}\left(K_3\frac{\partial\theta}{\partial x_3}\right)\right] = h_p' - h_p \qquad (4.15)$$

Only the spatial and temporal distribution of the additional heat source $(h_p' - h_p)$ is required to integrate Equation (4.15), and the details of radiation attenuation and surface convection can be ignored.

When the definition of excess temperature is applied to the sectionally homogeneous relation, Equation (4.9), it yields

$$\left[\frac{\partial \sigma\theta}{\partial t} + \frac{\partial}{\partial x_1}(u_1 \sigma\theta) - \frac{\partial}{\partial x_1}\left(\sigma D_1 \frac{\partial \theta}{\partial x_1}\right)\right] = -\frac{W \cdot K}{\rho c_p}\theta \tag{4.16}$$

Equation (4.16) is independent of the equilibrium temperature E and consequently much of the detailed meteorological data required for evaluation of surface heat exchange processes.

The temperature $T(x_i,t)$ can be considered the ambient temperature relative to the temperature excess $\theta(x_i,t)$. The conservation expression for excess temperature, Equation (4.15), is valid in a region of the waterbody for which the spatial gradients of ambient temperature $\partial T/\partial x_i$ are small in comparison to the spatial gradients of excess temperature $\partial\theta/\partial x_i$. This condition is usually satisfied in the immediate vicinity of a large heat source where the consistency of velocity field and dispersion field is violated. Linearity of the equation for temperature excess permits the separate determination of the temperature excess distribution for each individual thermal discharge and superposition of the results.

3.2 INITIAL TEMPERATURE DISTRIBUTIONS

The temperature distribution in the immediate vicinity of a discharge is a function of the discharge structure design. The advective and dispersive field transporting heat in this region is determined by the momentum and buoyancy of the discharge, as these dominate the advective and dispersive properties of the receiving waterbody. Currents and stratification in the receiving waterbody eventually dictate the limits of initial mixing.

A classification of initial mixing conditions based on recent representative studies is given in Table 4.1. Discharge characteristics are categorized as surface-buoyant, surface-non-buoyant and submerged-buoyant discharges. Receiving waterbody characteristics are classified as stratified and nonstratified, and according to the presence or absence of a current. The non-buoyant surface discharge cases should be further subdivided into two-dimensional and three-dimensional plumes, indicating the number of directions over which a jet could expand.

Thermal discharges have a high momentum because of their large volume flow rate. As momentum is transferred to the receiving waterbody, large volumes of ambient fluid are entrained, thus diluting the excess temperature. Entrainment is limited by the ability of ambient water to move into the discharge region and by the number of spatial directions in which the discharge expands. Bottom and shoreline topography can therefore limit the dilution achieved by the discharge momentum.

Historically the application of momentum jet theory has been in the study of wastewater outfalls. Its extension to thermal discharges requires recognition of two fundamental differences. First, most waste discharges require dilution factors on the order of 50:1 to 500:1 while thermal discharges require dilution factors on the order of 10:1. Second, waste

Table 4.1 Classification of initial mixing conditions and representative studies.

DISCHARGE CHARACTERISTICS

RECEIVING WATERBODY CHARACTERISTICS		Surface		Submerged
		Buoyant	Nonbuoyant	(Buoyant)
Nonstratified	No Current	Jen et al. (1966) Tamai et al. (1969)	Yevdjevich (1966)	Albertson et al. (1948) Abraham (1965) Fan and Brooks (1966)
	Current		Carter (1969)	Fan (1967)
Stratified	No Current	Harleman and Stolzenbach (1967) Rigter (1970)		Hart (1961) Fan (1967)
	Current	Wada (1967b)		

discharges are of relatively low volume compared to a thermal discharge. A practical summary of momentum jet relationships applicable to the study of initial mixing has been given by Wiegel (1964). Utilizing the method of dynamic similarity (Townsend 1956), it can be shown that for a jet expanding in two directions (laterally from the axis and downstream) the characteristic velocity will decrease with the square root of distance along the axis, and that for a jet expanding in three directions (laterally and vertically (or radially) and downstream) the characteristic velocity will decrease linearly with distance.

A fundamental property of momentum jet relations is that they are scaled directly to the geometry of the discharge orifice or structure. Thus, the following scaling relations can be established:

(i) Conservation of momentum along the jet axis

$$Q(x)U(x) = Q_o U_o \tag{4.17}$$

where $U(x)$ is the characteristic jet velocity at a distance from the discharge, $Q(x)$ is the flow within the jet at a distance from the discharge, U_o is the discharge velocity, and Q_o is the discharge flow rate.

(ii) Dynamic similarity of the mean velocity field and the root-mean-square (turbulent) velocity field, which dictates that for a two-dimensional plume

$$\frac{U_2(x)}{U_o} = \left[\frac{x_{o2}}{x}\right]^{\frac{1}{2}} \qquad (4.18)$$

and for a three-dimensional jet

$$\frac{U_3(x)}{U_o} = \frac{x_{o3}}{x} \qquad (4.19)$$

where $U_2(x)$ signifies the two-dimensional longitudinal characteristic velocity and x_{o2} the two-dimensional virtual source position; and $U_3(x)$ signifies the three-dimensional longitudinal characteristic velocity and x_{o3} the three-dimensional virtual source position.

Combining the characteristic velocities with the conservation of momentum in the jet, Equation (4.17), leads to the dilution flow relations of

$$\frac{Q_2(x)}{Q_o} = \left[\frac{x}{x_{o2}}\right]^{\frac{1}{2}} \qquad (4.20)$$

for a two-dimensional plume, and

$$\frac{Q_3(x)}{Q_o} = \frac{x}{x_{o3}} \qquad (4.21)$$

for a three-dimensional plume. For jet discharges, the virtual source distance is about two to ten times the diameter or width of the discharge orifice. An important result of the above analysis is that the dilution ratio $Q(x)/Q_o$ is constant with distance. Therefore, doubling the discharge rate through the same discharge structure doubles the entrainment and should lead to the same dilution at the same distance from the discharge.

Dynamic similarity does not dictate the shape of the velocity profile perpendicular to the jet axis. This shape must be inferred from observation and it has been the practice based on laboratory experimentation to assume a Gaussian function. Pritchard (1970) indicates that a rectangular or "top hat" distribution may be more appropriate for large volume flow rate thermal discharges. Extension of the dynamic relations to contaminant distributions is based on the assumption that contaminant concentrations will follow the same distribution axially and radially as the velocity distribution. Concentrations will therefore decrease with the square root of distance for a two-dimensional jet and decrease linearly with distance for a three-dimensional jet.

Buoyancy of a horizontal surface momentum discharge tends to retard the rate of vertical mixing and results in greater lateral spreading than for a nonbuoyant horizontal discharge (Jen et al. 1966 and Tamai et al. 1969). Consistent with the dimensional relations of dynamic similarity, it is assumed that the axial concentration for a buoyant jet decreases linearly with distance as for the three-dimensional nonbuoyant case. It has been necessary, therefore, to incorporate the influence of buoyancy empirically into the lateral distribution function.

The influence of ambient currents and receiving waterbody stratification on surface jet discharges presents a large number of possible situations. Pritchard (1970) suggests that if a longshore current is large compared to the normally directed velocity of a jet, then the plume can be bent toward the shoreline and entrainment of the shoreward side of the plume would be inhibited. When a highly developed thermocline exists it is possible that vertical entrainment will be inhibited to such an extent that a three-dimensional jet discharge will degenerate to a two-dimensional laterally spreading configuration. In the case of an estuary with a strong halocline, it is possible that a condenser temperature rise will produce a density only slightly less than exists for the surface waters with the result that a plume will plunge below the surface after limited entrainment. In addition, Abraham and Kondstall (1969) have presented data showing the influence of surface winds in distorting surface temperature distributions.

Dilution by a momentum discharge subjected to an oscillating current must also be considered. Momentum of the jet relative to the receiving waterbody would be large during slack water, but the reverse may be true during ebb and flood current conditions with the result that jet entrainment may be ineffective during these periods. The domination of ebb and flood current momentum over discharge momentum can lead to large "globs" of heat (scaling tens of feet) being broken away from the plume. Large ebb and flood currents will, however, provide the "new" dilution water necessary for entrainment. It appears insufficient to say that momentum mixing terminates where jet velocity matches current velocity. Rather, it appears necessary to match jet momentum to waterbody momentum including not only the mean current velocity but also the current shear.

Submerged buoyant jets have been studied extensively for application to waste discharges, and relations dictating their major properties are well established (Fan and Brooks 1966). They are characteristically three-dimensional up to the point of interference between individual jets. Comparison of submerged buoyant jet relations to the high volume flow rate discharges of thermal power plants has not yet been accomplished. The submerged buoyant jet, as well as the surface jet, provides the source distribution of temperature relative to larger scales of mixing.

3.3 INTERMEDIATE TEMPERATURE DISTRIBUTIONS

Temperature distributions outside the region of momentum mixing are governed by the advective and dispersive field of the receiving waterbody. The temperature distribution in the intermediate region can be estimated no more precisely than the detail with which the velocity field and dispersive field can be specified for inclusion in the heat conservation relation, Equation (4.15). The velocity field is no longer dictated by discharge characteristics but must be inferred from the equations of motion applied to large segments of the waterbody.

Relative to the intermediate temperature distributions, the initial temperature distribution determined by momentum mixing acts like an extension of a thermal plant condenser. The distribution resulting from initial mixing, either by surface or submerged discharges, gives the source distribution to be used as one boundary condition in the heat continuity relation. When a large fraction of dilution is achieved by momentum mixing, there is little to be accomplished in the intermediate mixing processes.

In order to provide relationships for establishing the relative size of plant discharges to waterbody characteristics, Edinger and Polk (1969) have summarized solutions to the heat conservation relation assuming lateral, and lateral and vertical dispersion of heat from a point source into a uniform current. These relationships are represented as the surface area within a given temperature excess contour, in order to provide a rapid method for analyzing large amounts of observational water temperature data. With such an oversimplified representation of the velocity field, dispersion, and boundary conditions, the surface area within contours is about as detailed a description of the temperature distribution as is practical. For a three-dimensional distribution the scaling relation between surface area and temperature excess is approximately

$$\frac{A}{A_{n3}} \approx 0.496 \left(\frac{\theta}{\theta_p}\right)^{-3/2} \qquad (4.22)$$

Here A is the surface area contained within a contour of temperature excess θ, θ_p is the temperature excess after momentum mixing, and A_{n3} is a scaling area given as

$$A_{n3} = 0.178 \frac{Q_p^{3/2}}{U^{1/2}\ D_y^{1/4}\ D_z^{3/4}} \qquad (4.23)$$

in which Q_p is the dilution flow after jet entrainment, U is the uniform current velocity, D_y is the lateral dispersion coefficient, and D_z is the vertical dispersion coefficient. In the case where there is no momentum mixing at the discharge, Q_p and θ_p would be the plant pumping rate and condenser rise respectively. For a two-dimensional distribution which is vertically mixed the scaling relationships become

$$\frac{A}{A_{n2}} = 0.168 \left(\frac{\theta}{\theta_p}\right)^{-3} \qquad (4.24)$$

where the scaling area A_{n2} is defined as

$$A_{n2} = 0.715 \frac{Q_p^{3}}{D_y\ U^2\ d^3} \qquad (4.25)$$

where θ_p, Q_p, D_y, and U are as previously specified and d is the thickness of the vertically mixed water column. In the above scaling relations, it is significant to note that the area increases with the 3/2 power of the plant pumping rate for the three-dimensional case and with the cube of the plant pumping rate for the two-dimensional case.

The vertically mixed case was extended to include the influence of surface heat dissipation and it was found that there was little reduction in area for contours of temperature excess greater than 0.2 θ_p. A similar conclusion on the relative influence of surface cooling during initial and intermediate mixing stages has been reached by Pritchard (1970).

The three-dimensional intermediate mixing relation was extended to include the cross-sectional area within a temperature excess contour as a function of distance from the discharge. These relations indicate that the section area within an isotherm should increase as the

$\ln(\theta_p/\theta)$ at each cross section, which agrees with the data plots of Lawler and Leporati (1968) for a thermal discharge on the tidal reaches of the Hudson River.

Description of surface area within a temperature excess contour represents the present empirical detail for scaling large heat sources to receiving waterbody size. A unique relationship between initial and intermediate mixing relations can be developed for the two-dimensional cases which shows the area A_m and the temperature excess θ_m where the two match. Beginning with Equation (4.20), the "width" of the two-dimensional jet can be defined as

$$b(x) = \frac{Q_o}{U_o d} (x/x_{o2}) \qquad (4.26)$$

the distance from the discharge to a $\theta(L)$ contour is given by

$$L = x_{o2} (\theta_p/\theta_L)^2 \qquad (4.27)$$

and the surface area in this contour becomes

$$A_L = \int_o^L b(x)\, dx = \frac{Q_o\, x_{o2}}{U_o\, d} (\theta_p/\theta_L)^4 \qquad (4.28)$$

and

$$\theta_L/\theta_p = (x_{o2} Q_o/U_o d)^{\frac{1}{4}} A_L^{-\frac{1}{4}} \qquad (4.29)$$

Now, Equation (4.24) gives the intermediate surface area for a two-dimensional distribution. Equating (4.24) to (4.29), the area A_m where jet dilution matches intermediate mixing is found as

$$A_m = (2.07 \times 10^{-4})\, Q_o^9\, U_o^3\, D_y^{-4}\, U^{-8} d^{-9} x_{o2}^{-3} \qquad (4.30)$$

The temperature excess around this area, from (4.29), would be

$$\theta_m = \theta_p (x_{o2} Q_o/U_o d)^{\frac{1}{4}} A_m^{-\frac{1}{4}} \qquad (4.31)$$

Thus the area at which two-dimensional jet mixing matches two-dimensional intermediate mixing increases as the ninth power of the plant pumping rate Q_o and as the cube of the jet velocity U_o which are two variables at the control of the designer. This makes the question of designing a condenser cooling water system for low Q_o and high θ_p or high Q_o and low θ_p one one of the most important facing the industry today. The biologist concerned about organism entrainment and pump damage would probably prefer a low Q_o (L. L. Jensen, personal communications). Similiar relations can be developed for the three-dimensional cases once the form of the lateral temperature equation is assumed.

Other analytic studies of intermediate mixing have been conducted. Wada (1967) has provided a numerical integration of the heat conservation relation for an assumed uniform current, a temperature-density dependency on the dispersive terms, a specified ambient temperature stratification downstream of the discharge, and rectangular discharge boundary configuration. Pritchard and Carter (1965) have predicted the temperature excess distributions based on in situ dye measurements by assuming similarity between the conservation of dye and conservation of excess heat. These predictions were later compared to prototype conditions by Carter (1968).

The amount of mixing that can be achieved in a waterbody of finite extent is determined by large-scale circulation. In the simple case of a river, for example, the upper limit to dilution is set by the river flow. In tidal and estuarine situations the detail with which the fully mixed conditions can be defined depends on the detail with which the large-scale tidal circulation is modeled.

3.4 LARGE-SCALE TEMPERATURE DISTRIBUTIONS

Problems of formulating large-scale temperature distributions in estuaries have been discussed in Sections 1 and 2 of this chapter. This discussion concerns the superposition of temperature excess due to a single source in large-scale models. It is at this large scale that dissipation of excess heat to the atmosphere becomes important. However, depending on the relative size of a thermal discharge to large-scale circulation, the fully mixed temperature excess will usually be negligible compared to the temperature excess in the initial and intermediate mixing regions.

Analysis of large-scale temperature distributions presumes the existence and verification of a water quality model for other water quality parameters such as salt, dissolved oxygen or BOD. The spatial and temporal detail with which excess heat can be modeled is predetermined by the nature of the existing water quality model. There is no independent temperature distribution model since heat obeys the same conservation relations, at least in the advective and dispersive processes, as the other water quality parameters. Exceptions have been discussed in Sections 1 and 2 where it is indicated, for example, that a vertically homogeneous or sectionally homogeneous salt distribution does not necessarily imply a priori a similar vertical distribution of temperature.

Explicit, but simplified, continuity relations for a heat source relative to large-scale distributions can be written for the sectionally homogeneous and the two-layered segmented cases discussed in Section 2. This is possible because the advective terms in these models can be inferred. Empirical requirements for inserting heat sources in segmented models are examined in this section. For geometrically complex large-scale models, the excess temperature distribution after intermediate mixing becomes the source distribution, and if the large-scale model includes the details of velocity and dispersion over the scale of intermediate mixing then the source distribution is determined by initial mixing conditions.

Consider the sectionally homogeneous case. The excess heat balance is given in Equation (4.16). Assuming that the excess heat balance is averaged over a time period so that the local heat storage term is negligible, the "steady-state" heat balance for a short segment of the estuary becomes

$$Q \frac{\partial \theta}{\partial x} - \frac{\partial}{\partial x}\left[(\sigma D_l) \frac{\partial \theta}{\partial x}\right] = - \frac{WK\theta}{\rho c_p} \qquad (4.32)$$

where Q is the advective flow through the segment found by averaging the product of cross-sectional area and velocity over the same time period that makes the heat storage term negligible. Q is often taken as the freshwater inflow. It is implicit that additional cross-product terms $(\langle u_1'\theta'\rangle)$ are now incorporated in the longitudinal dispersion coefficient as a result of this averaging. If it is further assumed that Q and σD_1 are constant over a segment near the source (located at $x = \ell_s$), then the time-averaged sectionally homogeneous heat balance equation has the solution near $x = \ell_s$ of

$$\theta = \theta_1 e^{a(x-\ell_s)} + \theta_2 e^{b(x-\ell_s)} \tag{4.33}$$

where

$$a = \tfrac{1}{2}\left[Q/\sigma D_1 + \sqrt{(Q/\sigma D_1)^2 + (4WK/\rho c_p \sigma D_1)}\right] \tag{4.34}$$

and

$$b = \tfrac{1}{2}\left[Q/\sigma D_1 - \sqrt{(Q/\sigma D_1)^2 + (4WK/\rho c_p \sigma D_1)}\right] \tag{4.35}$$

and where θ_1 and θ_2 are constants of integration. For $x > \ell_s$, $\theta_1 = 0$ for θ to decrease with distance and

$$\theta = \theta_s e^{b(x-\ell_s)} \quad \text{for} \quad x > \ell_s \tag{4.36}$$

where θ_s is the fully mixed sectionally homogeneous temperature near $x = \ell_s$ which is yet to be evaluated. Similarly for $x < \ell_s$, $\theta_2 = 0$ for θ to decay away from the source, hence

$$\theta = \theta_s e^{a(x-\ell_s)} \quad \text{for} \quad x < \ell_s \tag{4.37}$$

The rate at which heat is discharged at a source H_s must be just equal to the rate at which heat is advected and dispersed upstream and downstream, assuming no heat dissipation over the area required to achieve complete mixing. Since there is no net advection of heat through the sectionally homogeneous segment, the heat balance relative to the source becomes

$$H_s = \rho c_p \sigma D_1 \left(- \frac{d\theta}{dx}\bigg|_{x=\ell_s^-} - \frac{d\theta}{dx}\bigg|_{x=\ell_s^+} \right) \tag{4.38}$$

and using Equation (4.36) and (4.37) to evaluate the upstream and downstream gradients, then

$$H_s = \rho c_p D_1 \ \theta_s (a - b) \tag{4.39}$$

or

$$Q_s = \frac{H_s}{\rho c_p Q \sqrt{1 + (4W\sigma D_1 K/\rho c_p Q^2)}} \tag{4.40}$$

which relates source strength H_s and fully mixed temperature excess θ_s. In this case, the fully mixed temperature excess θ_s represents the limit on mixing that can be achieved by the initial and intermediate process. Thus, in the end, the initial and intermediate mixing processes cannot be completely independent of surface heat exchange.

Sectionally homogeneous relationships, similar to those above but modified for net downstream advection and upstream boundary reflection, were applied by Edinger and Geyer (1968) to a thermal discharge in a narrow tidal embayment. Results of this analysis, shown in Figures 4.5-4.7, are presented in terms of dimensionless parameters for ease of scaling to different plant and embayment conditions. The advective flux could be explicitly identified with the plant pumping rate since the plant intake was from a source other than the embayment receiving the discharge. The temperature rise was measured from the equilibrium temperature rather than the temperature distribution before addition of excess heat because of the significant change in the advective field due to the discharge. It was found that the "steady-state" sectionally homogeneous heat balance matched mean monthly temperature averages of weekly observations during the July period for two different plant loadings. Considering the number of assumptions involved in arriving at the sectionally homogeneous relations and the uncertainty of the time-averaging procedure involved, Equation (4.40) can be considered at best a crude estimate of fully mixed temperature excess.

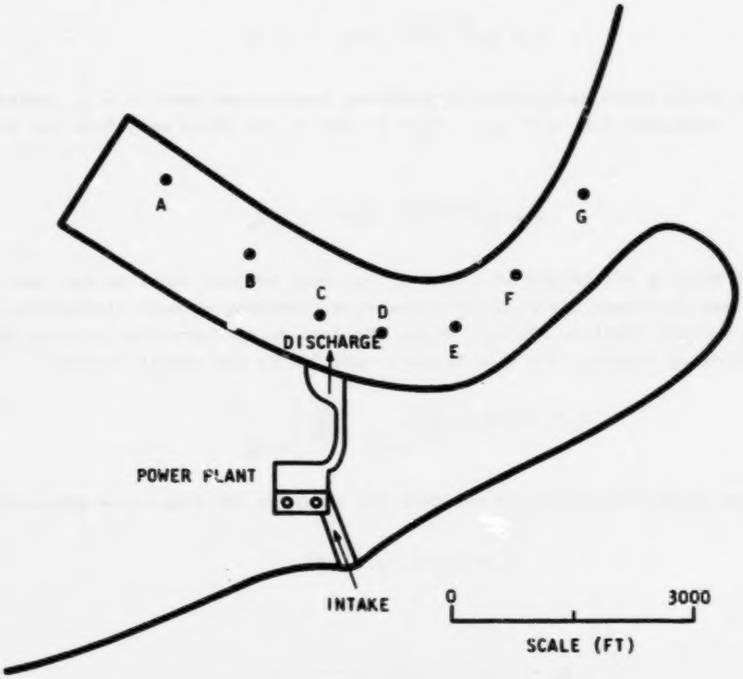
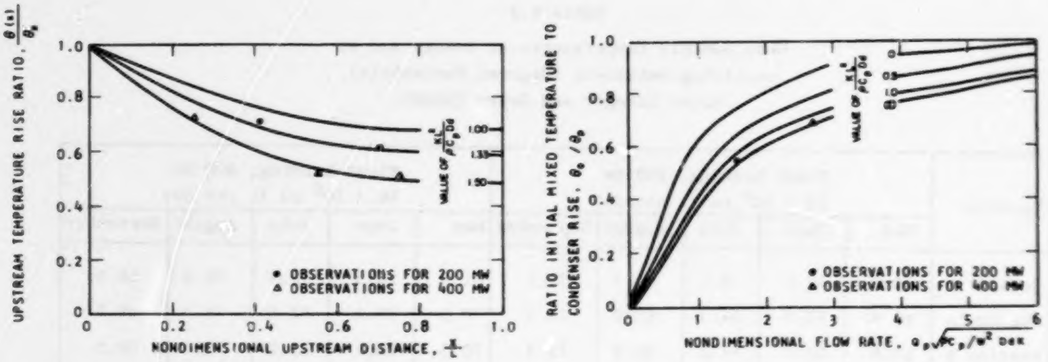
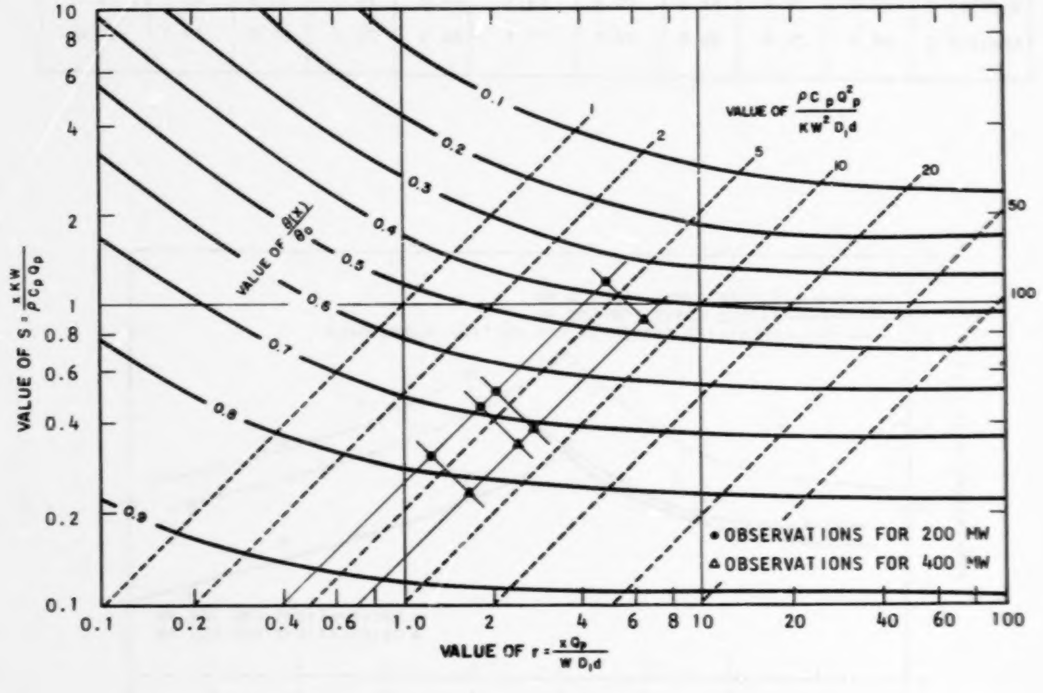


Fig. 4.5 Location map, power plant discharge area. From J. E. Edinger and J. C. Geyer, Analyzing Steam Electric Power Plant Discharges, Proc. ASCE, 94, No. SA 4 (August 1968), pp. 611-623. Used with permission of the American Society of Civil Engineers.



(a) Upstream temperature distributions.

(b) Initial temperature rise ratio as function of plant discharge rate.



(c) Downstream curves of constant temperature rise ratio as function of nondimensional coordinates.

Fig. 4.6 Nondimensional forms of one-dimensional analysis. From J. E. Edinger and J. C. Geyer, Analyzing Steam Electric Power Plant Discharges, Proc. ASCE, 94, No. SA 4 (August 1968), pp. 611-623. Used with permission of the American Society of Civil Engineers.

Table 4.2

Mean monthly temperatures at intake and in receiving embayment (degrees Fahrenheit). After Edinger and Geyer (1968).

Location	Plant Loading, 200 Mw 23×10^6 cu ft per day					Plant Loading, 400 Mw 46×10^6 cu ft per day				
	May	June	July	August	September	May	June	July	August	September
Intake, T_i	70.5	77.8	78.1	77.5	70.5	61.8	74.3	78.2	76.0	66.5
Station A	68.8	80.0	81.3	81.0	73.5	70.5	79.5	81.8	79.3	68.0
Station B	69.0	80.0	81.8	80.9	73.3	70.5	80.2	82.0	76.6	68.5
Station C	70.0	81.5	83.4	81.4	74.3	71.8	81.5	83.5	81.9	72.3
Station D	70.0	80.8	82.8	82.4	75.5	71.5	81.8	85.2	83.2	74.0
Station E	69.0	79.8	81.4	81.3	74.7	68.3	80.0	84.7	82.7	71.3
Station F	69.0	79.8	81.3	80.9	73.5	68.0	79.0	83.8	80.5	71.3
Station G	68.5	79.0	80.0	78.9	72.5	66.5	76.0	82.0	79.7	70.0

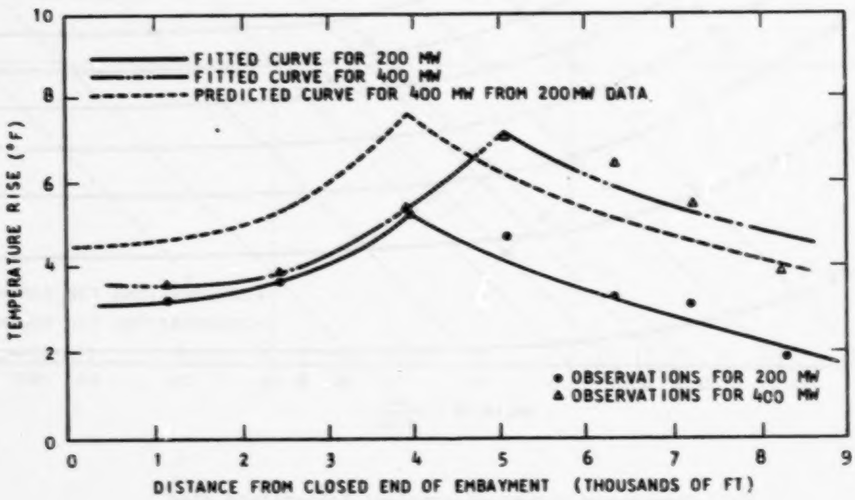


Fig. 4.7 Longitudinal temperature distributions for case study. From J. E. Edinger and J. C. Geyer, Analyzing Steam Electric Power Plant Discharges, Proc. ASCE, 94, No. SA 4 (August 1968), pp. 611-623. Used with permission of the American Society of Civil Engineers.

Table 4.3

Parameters from fitted data. After Edinger and Geyer (1968).

Parameters	200 Mw operation	400 Mw operation
Plant pumping rate Q_p (cu ft per day)	26×10^6	52×10^6
Distance to closed end L (ft)	3,900	5,100
Thermal exchange coefficient K (Btu ft per day per °F)	155	144
Upstream apparent diffusivity D_2 (sq ft per day)	7.0×10^6	10.0×10^6
Downstream apparent diffusivity D_1 (sq ft per day)	3.76×10^6	4.6×10^6

Magnitudes of fully mixed temperature excess given by Equation (4.40) for the Delaware River-Estuary based on values of longitudinal diffusivity and river geometry tabulated by Pence et al. (1968) are shown in Figure 4.8. The result is given in terms of °F rise per 10^9 Btu hr^{-1} of waste heat rejection and is presented here only to indicate the magnitude of heat sources relative to a particular waterbody, which has been the subject of discussion elsewhere in this report. The transition from dilution by river flow alone to that provided by dispersion and increased geometry with distance is illustrated. A more satisfactory estimate of fully mixed concentrations would be based on Equation (2.148) of Chapter II which accounts for velocity variations within a tidal cycle and eliminates the difficulty of interpreting the temporal averages of Q and D_1 .

For segmented and multilayered models, as discussed in Section 2.2 of this chapter, Equations (4.10) and (4.11), the source flux ($H_s/\rho c_p$ in these equations) is added to the heat balance for the segment at the point of discharge in a manner similar to that indicated by Pritchard (1967). Implied are the conditions that (1) initial mixing and intermediate mixing are complete within this segment, (2) momentum entrainment only influences circulation within the segment but not across segment boundaries, and (3) intake-to-discharge circulation takes place within the same segment. The first condition might be satisfied empirically if the surface area of the segment is larger than required to give the average segment temperature rise based on the intermediate distribution relationships of Section 3.3. The second and third conditions are related to modification of the overall circulation pattern by the large volume flow rate of a thermal source. An imputed circulation pattern based on the continuity of salt cannot be readjusted by mass continuity relations alone, but will require additional approximations based on momentum conservation. However, the second condition might be satisfied if it can be assured that the flow required to dilute the condenser temperature rise to

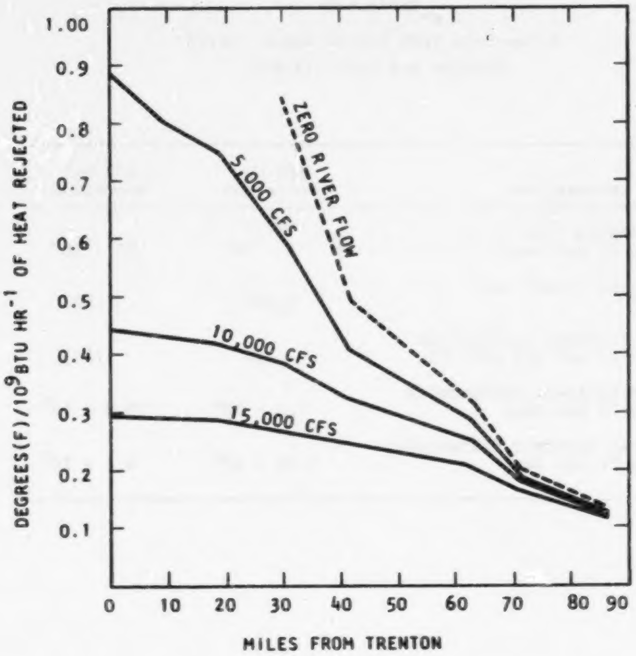


Fig. 4.8 Fully mixed temperature at point of discharge for a single plant at any location. Based on Delaware River-Estuary data of Pence et al. (1968)

the fully mixed temperature rise of the segment is much less than the total advection into the segment. The third condition may not be physically possible in the case of a submerged intake and surface discharge, each in separate segments, or in the case of a submerged buoyant discharge, but if the plant pumping rate is small compared to the vertical flux between the segments it might be neglected. It will be necessary, however, to ensure that buoyant convection due to combined temperature-salinity density differences between the intake and discharge presents no problem.

3.5 PHYSICAL HYDRAULIC MODELING OF THERMAL DISCHARGES

The inability to provide sufficient detail of the velocity field in segments of a waterbody near a thermal plant site has lead to the use of physical hydraulic models to simulate intermediate and initial mixing conditions. Principles and practices of hydraulic modeling are discussed thoroughly in Chapter V. Comparison of model results to prototype conditions for a number of thermal discharges have been presented by Ackers (1969). Problems of hydraulic model construction and calibration for thermal discharges are discussed by Jeffers et al. (1969).

A detailed comparison of model results and analytic descriptions of initial and intermediate mixing processes of a thermal discharge have been presented by Harleman and Stolzenbach (1969). The model is scaled according to a densimetric Froude number criterion, a beach slope and discharge channel aspect ratio criterion based on the work of Wiegel (1964), and a surface cooling criterion based on the results of Hayashi and Shuto (1967). The Froude criterion establishes the velocity and depth scale $(V_r = h_r^{1/2})$, and the surface cooling criterion used in this study establishes the length and depth scale $(L_r = h_r^{3/2})$. With distortion in the model the slope criterion of Wiegel cannot be satisfied. Results of the model are compared to the initial mixing behavior of a three-dimensional jet (where dilution increases linearly with distance) and it is found that jet mixing dominates to a distance of thirty times the discharge width. Beyond this distance, where temperature rise is about two-tenths the condenser rise, it is concluded that surface cooling begins to be important.

Future progress in the quantification of the complex temperature distributions surrounding thermal discharges requires a combination of hydraulic and analytic modeling coupled with prototype studies. In the past, analysis has dictated the scaling of hydraulic model results to prototype conditions, but it appears that the future direction must be reinforcement and verification of analytic solutions (which are now becoming quite complex) by hydraulic modeling and then extension to more variable prototype conditions through analytic methods.

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DISCUSSION

EDINGER: My approach was to begin with the assumption that there is no single water temperature model for an estuary, and proceed to look at how many different formulations can be developed from continuity relations. It is recognized that we cannot determine the temperature distribution in an estuary in any more detail than we know the velocity field, both temporally and spatially, hence the temperature models are very dependent on dynamic models. In the first two sections are discussed large-scale natural temperature distributions with ambient conditions at a river and ocean end and surface heat exchange but no major sources in the middle. So the argument is that, first of all, we consider that the heat conservation relation and the salt conservation relation will be the same in the advective, storage and dispersive terms, and this will lead to some similarity between salinity distributions and temperature distributions, and any deviation in this similarity will be related then to surface heat exchange and a number of other factors. The fact is here that you have the same transport relationships, and the boundary condition of zero salinity at the river end can be made compatible to zero enthalpy at the river end by using the river end temperature as a base temperature from which to make your similarity arguments. The next step is to superimpose upon this, then, what we think might happen with incorporating surface heat exchange. This then lets us intuit or sketch out what we might expect for longitudinal temperature distributions. These are shown on Figure 4.3.

We then come to two very important problems that make heat difficult to handle in the analysis of temperature distribution. The first is the problem of attenuation of shortwave radiation with depth and through the water column. Most of our knowledge on the relationships of shortwave radiation attenuation and vertical temperature structure is presently derived from freshwater lake type models. The fact is, though, in some situations, with high salt concentrations in deep layers and even in winter months, we can have high temperatures in lower layers due tc absorption of shortwave radiation.

The second problem is what do we do with the surface boundary condition necessary to account for attenuation of shortwave radiation through the surface in a vertically varying temperature structure. I have written in Equation (4.6) a fairly general statement to show that the rate at which heat has to be transported away from the water surface is related to the vertical dispersion at the water surface, as well as some buoyant convection which is related to the velocity field. This, I might point out, is following the discussions that Phillips brings to bear on the problem of vertical convection at the surface. It becomes clear that if for any reason we can assume heat uniformly mixed through the vertical in the water column, there is no problem as far as temperature prediction is concerned. The question is whether this is valid. It seems to me that we are going to have to be incorporating in a temperature model, particularly when we want detail in the vertical temperature structure, some type of computational process, similar to that used by Dake and Harleman, to account for convection of heat near the water surface. In the case of the estuary, we are going to have to make the convective computations dependent on salt concentration as well as temperature, but it won't be too much of a problem, because I do not think we are going to affect the salt distribution that much in the initial calculations.

The third section of this chapter deals with temperature distributions due to large heat sources. Generally we have discovered that we have to consider three spatial scales in classifying present analytic techniques. One is an initial mixing region near the discharge which is a function of discharge design. Secondly, there is an intermediate region where the heat is tending toward the larger scale distribution. Third, there is the large-scale temperature distribution which we might consider to be the longitudinal and vertical temperature distribution resulting from the large heat source.

These three regions then, right at this stage, are described by independent analytic methods. I think we are in a situation where we need some simple scaling relationships to tell us how big or small each region is in a particular type of water body. We find that most of the research that has been done and published in this field has not been directed explicitly towards high volume, high momentum, low concentration discharges like we have with heat. That is, for initial mixing of discharges, most of the work has been directed towards sewage discharges which have low volume, very high concentrations, that require dilutions in the order of a hundred or a thousand to one, and with heat we are not looking for much more than five or ten to one in the way of dilution. Also not much of the work has been done in the field directly with power plants themselves.

RATTRAY: The part of this that I have had a chance to look at here, I go along pretty well with. These segmented models bother me, but I'm not the only one.

EDINGER: They do me, too. Well, this is a fairly common one that is used, and the thing that I am pointing out here is that it is not too difficult a trick to turn this into a temperature model if you want. We don't have to derive a new segmented model if we accept this one, you see.

RATTRAY: There is one place I had trouble on something that seems to be fairly commonly understood and maybe I don't understand. And that is in salt-wedge estuaries. It is in here and other places too, about net upward advection out of the salt wedge. I just don't really have a very good feel for that. I suspect the salt exchange between the wedge and the fresh water is a practically negligible quantity. That's what I am asking.

PRITCHARD: Depending upon what you define as a salt-wedge estuary. If you take something that doesn't exist and call it a salt-wedge estuary, you might be right. But if you take the real systems which we classify as salt-wedge, like the Mississippi, then you have the water surface, the bottom, and the wedge coming in here as a fairly well-defined gradient in salinity. The main difference between a salt-wedge and a moderately mixed estuary is that there is no dilution of water in the wedge. That is, this is ocean concentration all the way up the mouth and is defined almost like a front, but an exchange does occur with a transport of salt into the fresh water, and you can see that gradient, the salinity increasing.

From his flume work, Keulegan showed at this interface there is a velocity difference between the underlying wedge and the top layer, and you get interfacial waves, and these interfacial waves break. They always break upwards, so even that though this looks like turbulence you are really transporting both salt and water. You find the wedge is constant for constant river flow, and since you are passing salt upwards you've got to have flow inwards. Admittedly, this is very much smaller. It's like equal to the river flow or something like that, rather than several times the river flow. That is, the volume of water coming in at the ocean end in the wedge is not an order of magnitude larger than the river flow as it is many moderately mixed estuaries.

RATTRAY: I just wonder how good the data are on that. I have tried to get Mississippi River data.

PRITCHARD: Most of this is from the Mississippi model, in fact.

VLASTELICIA: Have these waves been observed in the model breaking?

PRITCHARD: They've been observed in the flume. The original work was done by Keulegan, his study of instability in stratified flows. And it depends upon your terminology. I just don't know of any natural environment in which the salt-wedge comes in completely so that you have no gradient in salinity in the upper layer. Now it's true that for very low river flows, that salt-wedge goes up the Mississippi for a hundred-some miles and you are taking out fresh water out over the top of it. If you measure the salinity of it, it is slowly increasing seaward over the wedge.

RATTRAY: The rate of that increase is what really worries me, because if you talk about it as an advective flux, it should be fairly rapid. If it is a molecular diffusive flux, it should be very slow.

PRITCHARD: It's a matter of definition. And I define an advective flux as where you pass both water and salt, as distinct from where you just transport salt.

RATTRAY: It is possible to work out a balance that works very well in predicting salt-wedge shape and intrusion with nothing but molecular friction stresses at that boundary. So I don't know, because I haven't seen good data, but I raise the question.

EDINGER: The point of it is that I don't think it depends upon the reliability of the model, or whether we believe the existence of the salt-wedge estuary or not, but that there is a similarity between temperature and salt. The fact of it is that we certainly shouldn't be surprised to have longitudinal temperature distributions in an estuary, of what magnitude I am not sure yet, but I think at least we should expect it to vary seasonally. There will be times when there will be maximum temperatures and minimum temperatures throughout the longitudinal length, and this is mainly what I am trying to spell out. As a matter of fact, the same arguments about mixing colder water toward the surface would hold for the partially mixed estuary.

PRITCHARD: You just wouldn't have the bottom the same temperature as the ocean there.

EDINGER: That's right. The main thing is to have some type of framework in which to summarize it.

VLASTELICIA: What about extending the plume into the real time model at all in an estuary, in the distribution and its movement?

EDINGER: The thing that I point out here is that the status of the art is such that we're basically picking up simple descriptions of the sizes of these plumes case-by-case and then overlapping these. I don't think that we have any general model that will cover all these scales yet, and, even numerically, I don't think we will. I don't have a computation on this but my feeling is that we'll probably have as much computational difficulty determining the local temperature distribution right off the discharge as we will the large-scale distributions. I feel that the state-of-the-art is such that the problem of knowing when a momentum discharge condition ends and the larger scale dispersion takes over is not well-defined, and I don't think it will ever be well-defined because it is not that clear as to what it should be analytically. We only have a vague feeling about when we reach, shall we say, the sectionally homogeneous or laterally homogeneous condition. Anyway, each almost has to be done separately.

DOBBINS: What about whether you release it at the surface or release it at the bottom?

EDINGER: Yes, it's going to make a difference in the distributions. Certainly. There's no doubt about it.

PRITCHARD: I think the point that needs to be emphasized is that from a practical standpoint, you're now talking about much larger volume rates of flow. You're talking about thousands of cubic feet per second, which is very large compared to even a big city's municipal discharge. And the kinds of problems you face now become different. Natural diffusion and the natural mixing processes near the source are the things that, I would say, decrease that sewage discharge. The tidal oscillations, etc., that make the plume around a sewage discharge a relatively small volume have very little effect for some time on the distribution of temperature from such an outfall, because essentially you're starting with such a large volume source.

Schematically, if you look at a continuous point source release, you're starting with a delta spike in the distribution curve so that there is a high gradient for the diffusion to work on. So you see diffusion acting instantaneously to decrease the concentration curve as you move down the plume. But when you start with a large volume source--one way to picture it is a line source in which essentially the distribution is square--diffusion, even large-scale diffusion, can only act on the edges where there is a concentration gradient. You've got to move well down the plume before natural diffusion can affect the concentrations in the center.

So what you have to do is design so that you promote mechanical mixing, or augment the nature here. In other words, you need to find a site where there is high dilution volume available, and then find a way to use it by the design of the discharge. Now, of course, one design is just to make a large-scale diffuser that is the type that Brooks designs for the ocean. Generally, this is difficult to design for this kind of a waterway, so what you do is to depend on a single port of high velocity dilution--a high velocity discharge and momentum entrainment. And the amount of dilution you can get this way is still very large.

From a practical standpoint, your concern is with an area which is dominated by the dynamics of the discharge itself. You just never phase into the large-scale computer model except insofar as you want to know how one system might interact with the other in a large scale. Then I think you can sort of treat this case after the initial mechanical dilution has done some mixing, if you take multi-sources as already have been mixed in part and look at how they overlap with one of these larger scale, reduced-dimensional models. But the real problem that faces us today is what is the distribution around the outfall. I'm talking now within a tidal excursion of the outfall. This is where the decision is going to be made whether a plant meets the criteria or whether you're going to allow it to be in this estuary or not. It's not the large-scale distribution, but the distribution within a tidal excursion.

EDINGER: One of the problems is that in this intermediate region which I would consider to be the size of a tidal excursion or less, so to speak, the distribution you get depends solely upon your assumptions concerning the details of the velocity field. That is, if we know a two-dimensional time-varying velocity field in this region, that's the detail to which we can predict it. Whether we plug that amount of velocity detail into, say, a finite-difference calculation or not makes no difference: that's it. There is no sense in saying that different types of models are going to replace this.

PRITCHARD: I'd say except in the vicinity of the system where the dynamics are determined by the flow velocity of the jet itself.

EDINGER: That's right. This is what I've called the initial mixing region.

PRITCHARD: That probably occupies a sizable dilution zone, so that a significant part of the dilution is controlled by the dynamics of the discharge itself. There, of course, what you get out of it depends on what kind of model you take for the distribution of momentum within the jet.

CALLAWAY: In the third part there, you have something on temperature excess. How do you determine that?

EDINGER: Basically, temperature excess is defined as the difference between the temperature you have with a source and the temperature without it, both spatially and time varying. Within the immediate vicinity of a discharge, it doesn't seem to make much difference because your longitudinal temperature distributions probably wouldn't be that large.

PRITCHARD: Sometimes it does. For instance, I just looked at a Great Lakes situation where the temperature about 6,000 feet offshore varied from 48° onshore to 42° offshore. Your predictive technique predicts temperature excess, but then how do you apply it to this varied concentration offshore? It becomes a problem. In this case, one assumption one could make would be that the water being entrained into the jet has the mean ambient temperature between shore and the distance out to the point where you're making the prediction. Then you have to add your excess temperature to the mean of the sloping temperature curve between the discharge and the point at which you're making the prediction.

But it does get very difficult to talk about what is the base temperature, the ambient temperature. Particularly, if you just look at the real world, with no thermal plants on the waterway, and look at the temperature distribution spacewise and timewise in an estuary, they vary significantly. The problem of saying what is the base temperature if the plant weren't there, once it's there, is an extremely difficult thing. We've gone out and measured temperature distributions from heated discharges, and our biggest problem was to say how much of the temperature we're seeing is a rise above an ambient, because we couldn't pick the ambient very well. In the Patuxent River you can say to just put the measuring devices far enough away. But if you put them far enough away they vary very much anyway in time and space. Besides that, you can show that the plant affects the whole thirty miles of the estuary anyway. So it gets pretty difficult to do.

BAUMGARTNER: In answer to Dr. Dobbins' question, we, in another effort, have made a report on what models are available for ocean outfall design. We talk about the temperature models there. As Dr. Pritchard points out, you can come up with larger diffusers, but it's by no means technically or economically impractical to use them.

I have a question for Dr. Edinger. I just wonder in this chapter or some kind of summary, if you'll say something about how well these models can be applied to the types of situations we're concerned with now. Like if we had a model of Biscayne Bay for temperature distributions, or Puget Sound, or the Columbia River, or any other place you can think of. How well can we do that?

EDINGER: It would be my opinion that again it's only as good as the experience of the fellow who has worked with this particular set of calculations. I don't think any general rules can apply. Our state-of-the-art in terms of what formulations we have, or what few cases we can identify, isn't that good.

The one thing you can do roughly is that if you have an existing discharge, with some field observations, you can make some approximations about scaling that discharge to a different plant pumping rate and to a different heat rejection. This is within bounds, but won't be very precise. In other words, we can get from the continuity relations a few power scaling relations. There are many things we don't know about the coefficients on these. When I say we haven't had enough experience, it depends some days on how you feel, what you take for the scaling area or something.

BAUMGARTNER: You're saying you don't know how to measure α or b_c?

EDINGER: No, α and b_c are not the problem in local distributions. We are looking at entirely different types of relations. We're looking at relationships that involve some knowledge of the mean advective field that we haven't measured or predicted a priori. This we can at least get a picture of from an existing discharge. All our unknown constants, so to speak, are lumped in one place. So you can make a number of approximations, depending on what you want to assume for the type of discharge condition you expect, at least empirically, whether it's two-dimensional or three-dimensional, whether your entrainment will be limiting.

One important fact to keep in mind is that you can't entrain more water into the plume than you get to the edge of the plume. If anything limits the amount of water that can come in, it won't entrain any more. It will just keep on mixing on itself and you end up with a blob that disperses on through. These are embarrassing things to find out.

I think the state-of-the-art is that analysis is almost site-by-site. You can make some approximations as to whether a waterbody is large or small compared to a power plant, or vice versa, whether a power plant is large or small compared to a waterbody. Now, essentially we're doing this today for plants that will be looked at in detail seven years hence. If our guess is bad today, we're going to be in more Biscayne Bays seven years hence than we're looking at today. I would imagine the same thing has happened in many situations. The history of power growth has been that thousand-megawatt plants hit us almost overnight, with manufacturers coming out with a package unit within three or four years. We just weren't geared up to even know much about siting them, much less about the waterbodies in which they'd go. I see it not in terms of having a fixed formulation for all conditions. I see, rather, building up within individual utilities trained people who can look more critically at the siting problems and be familiar with waterbody hydrography. The better ones are doing this. And along with this, I think there is going to have to be some type of larger scale, more organized effort to pick the sites for the larger plants. After all there's going to be a finite number of them, and they're going to have to go someplace.

BAUMGARTNER: Is this an assessment that you mean to apply only to, say, the small scale or the intermediate scale problem? If you mean it to apply to the large-scale distribution, I think that's a materially different assessment than what I understand for, say, any other water quality constituent.

EDINGER: I think the thing of it is, if your power plant is so large in an estuary that it's going to influence the large-scale distribution, then the plant's probably too big.

PRITCHARD: I would agree that if it's really a problem on a large scale, if it's such a large problem, on a small scale it's impossible. It would be readily available with rather crude methods of prediction.

I'm more optimistic about what can be done now. I think that one can set general criteria for design, in terms of size, so that you would have said right off the bat that the size of the plant on Biscayne Bay is too big. And secondly, if you will accept not a detailed picture of the isotherms but such things as the area within having excess temperatures less than stated values, then, in fact, given a discharge design, the characteristics of the water, something about the longshore current distribution, one can predict the area contained within given isolines of excess temperature. You must decide whether you're going to predict a characteristic distribution or a 90% worst case or something like this. But for having made that statement, I think you're good within 25% or something like that on the average on the areas.

BAUMGARTNER: One last point. There has been some discussion that perhaps the water quality administrators cannot be satisfied with a worst case or a 90% prediction value, and they may want to have time distributions of temperatures, which might require joint probability distribution functions for evaporation effects, currents, winds, and variations on the heat loads. You may have seen in this first report that we talked a little bit about stochastic processes. I wonder if you would tend to include anything about that.

EDINGER: No, I don't, because I don't feel that this has developed far enough yet that we know enough about the statistics of water temperatures. A number of years ago, in '65, I set up the field studies for the Hopkins-EEI studies, and this was based upon the premise that the one thing that we could get at many different types of sites and the one thing that was needed was time-varying data. Unfortunately, it takes three years to get three years of time-varying data; and it still takes a few years and some people who are interested in time-variation statistics to start looking at it. I don't even think we know what type of statistics, so to speak, to crank into our model. I'm not sure what the status of the art is on this business; whether we have a deterministic model and can start cranking in time-varying conditions and get the calculated statistics out, or whether we should go back and redesign a model that's designed specifically to be a stochastic model. It's a rough question. It's an important one.

THOMANN: But I think that the point on stochastic aspects is very well taken, that you can run these models in a simulation-type framework with input statistics that generally represent what is occurring in the field environment. I think a fair amount of progress has been made in characterizing the statistics of some of these time series. Combinations of a few simple harmonics plus a regressive scheme can pretty well characterize some of the fluctuations. You can grind these into the deterministic model and take a look at the probability distributions of your output to answer those kinds of questions.

BAUMGARTNER: That answers one of them. You can simulate the conditions, if. But I think that you need to know something about the joint probabilities if you forecast.

EDINGER: Right, I think.

PRITCHARD: A comment. This is what has been observed in some records, not exceptionally long. But there has been some time series records taken in a way that one can sort of see what happens to an annual temperature curve, or the day-to-day temperatures over an annual cycle, with or without the plant there, by having recording thermistors at a location unaffected by the thermal plume--and, as I say, it's hard to know how far away you have to go. But we have some of these, which show, say, the annual pattern at that site removed from the plant site, watching the daily temperatures over a year's time. If you look at the distribution in the vicinity of the plant, what you see is the larger scale features, just the annual curve displaced. What one finds is in the spring the difference is somewhat greater than in the summer and winter, and during fall somewhat less. (Because during summer and winter the temperature is near equilibrium. During spring the equilibrium temperature is higher than the ambient temperature, and hence the cooling driving term is less than the difference between the heated temperature and the ambient. During fall the reverse is true.) But the major statistics of the two curves are the same, except for the mean value. All the higher moments than the first are essentially the same. So I'm just wondering whether one really needs to look at this. You want to know the stochastic character of the natural temperature variations from the biological standpoint. The imposition of the added heat term or added source term doesn't significantly change any of the moments of the probability distribution above the first.

EDINGER: What you're saying is pretty interesting in one sense, in that if you're talking about the statistics in natural temperature records, the best thing to analyze, by far, is the natural temperature record. But if all you're doing is playing the game and saying, "Well, I don't have a natural temperature record but I have a lot more meteorological data, so let's crank this in and then crank our flows into a temporal-spatial model and start cranking out answers on this," I'm still not convinced that there wouldn't be an awful lot of noise showing up in this calculation routine itself. An awful way to get water temperature records is to calculate them from meteorological data. We do everything we can to stay away from that.

CHAPTER V

PHYSICAL HYDRAULIC MODELS

Donald R. F. Harleman

1. INTRODUCTION

The earliest tidal models were built in Europe in the period 1875-85. In France, Fargue constructed a model to study the Garonne estuary from Bordeaux to the sea. In Britain, Osborne Reynolds used a tidal model to study shoaling and channel formation in the Mersey estuary. Reynolds' model had a horizontal scale ratio of 1/31,800 and a vertical scale ratio of 1/960, a distortion of 33 in the vertical direction. This was the first model in which the time scale for the tidal motion was related to the Froude condition for dynamic similitude for gravity and inertial accelerations. A summary of the history of tidal models, including a discussion of the important contributions of Osborne Reynolds, has been given by Ippen (1968).

In the United States, one of the first large tidal models was built in 1936 at M.I.T. by K. C. Reynolds (1936) for the Corps of Engineers. This was a model of the sea-level Cape Cod canal. The length scales were 1/600 horizontal and 1/60 vertical. This seems to have established the American practice of employing a vertical distortion of 10 in tidal models. Because of its responsibility for navigational facilities, the Corps of Engineers has played a leading role in the development of hydraulic model techniques at the Waterways Experiment Station, Vicksburg, Mississippi. During the last three decades, models of many of the estuaries of the East, Gulf and West coasts of the United States have been constructed. Motivation for the models has usually been problems associated with navigation improvements. In recent years many of these models have been used for the study of other problems including pollution and water quality. This has been due to an increasing awareness that navigation improvements may be detrimental to the multiple uses of an estuary. Wicker (1969) has classed estuary problems in the following categories:

Estuarine Problems

Due to Navigation or Navigation Improvements	Due to Factors Other Than Navigation
Channel Dimensions and Layouts	Effects of Land Fills
Shoaling	Effects of Bridges
Disposal of Dredge Spoil	Hurricane Surge and Tsunami Problems
Salinity Problems	Effects of Modifications of Upland Discharges
Effects on Shorelines	Effects on Shorelines

Changes in Regimen

Pollution

Problems Concerned with
Estuary Ecology

Changes in Regimen

Pollution

Problems Concerned with
Estuary Ecology

Aquatic Weeds

Physical hydraulic models have been used for the investigation of almost all of the problems listed above.

A tidal model is a much more complex and costly undertaking than its counterpart in the area of river and hydraulic structure models. Instrumentation is required for the transient measurement of water depths, velocities, and concentration of salinity, dye and other tracers. The reproduction of tidal motion at the model boundaries requires accurate control systems, and the boundary conditions are further complicated by the necessity of reproducing density differences associated with fresh water and saline ocean water. Light weight materials are often introduced to study scour and deposition patterns. A comprehensive survey of the use of hydraulic models in tidal waterway problems has been given by Simmons and Lindner (1965) and Simmons (1966 and 1969).

The reproduction of natural phenomena in a physical hydraulic model has an analytical basis in the theory of similarity. Traditionally, the derivation of the conditions necessary to achieve similarity is based on the concepts of *dimensional analysis*. This is a mathematical process of generating, as an output, a sequence of dimensionless groups from a set of input quantities which the engineer decides are important to the problem at hand. An objection to this approach is based on the fact that there is no well-defined procedure to guard against the inclusion of too few or too many input quantities. An alternative method, known as *inspectional analysis* (Birkhoff 1955), is recommended as a more rigorous approach to the theory of similitude. Inspectional analysis is based on the concept that there are certain physical laws which describe the flow processes. Usually they are stated in the form of differential equations related to momentum, heat and mass transfer processes. In a water quality model the set of differential equations would include the momentum equation of motion and a conservation of mass equation for each water quality parameter identified by concentrations of dye, salinity, BOD or dissolved oxygen.

Inspectional analysis is not concerned with the solution of the differential equations. Once the governing differential equations have been identified, the inspectional analysis is carried out by rewriting each of the differential equations in dimensionless form. This procedure will be illustrated in a later section. At this point it is only necessary to state that this results in certain dimensionless groups of physical quantities which appear as coefficients of various terms in the dimensionless differential equations. The principle of similitude can be started in the following manner: the fluid processes in two different systems, which are geometrically similar, will be identical if the dimensionless equations governing the fluid processes in the two systems are likewise identical. Since the governing equations are in dimensionless form, it is only necessary that the coefficients be numerically the same in model and prototype.

In physical estuary models, a difficulty arises from the requirement that the two systems (model and prototype) be geometrically similar. Non-geometric similarity, in the form of vertical scale distortion, is a characteristic feature of all physical estuary and tidal models. The necessity for vertical distortion becomes apparent when it is considered that the ratio of length to depth in a typical estuary may be of the order of 25,000. Thus a model depth of only 0.2 feet would require an undistorted model having a length of one mile. A model having the same depth and a vertical distortion of 10 results in a feasible length of approximately 500 feet. There is no exact analytical approach to dynamic similitude for distorted models. However, the need for vertical distortion is well recognized and non-controversial. In addition to feasibility in terms of space and operating personnel, vertical distortion is a means of avoiding prolonged periods of laminar motion during the tidal cycle, the increased water depths in the model result in better accuracy of depth and current velocity measurement, and undesirable capillary effects in the model are reduced.

The disadvantages of distortion may be summarized by observing that dynamic similarity is sacrificed to a certain extent, therefore reliability of the model results are more subject to question. It follows that the process of model verification, whereby the model is adjusted by trial to reproduce phenomena which were observed in the prototype, is a vital and necessary step. Physical models are built in order to study the effects of a proposed change in prototype conditions and it is important that the field data used for verification be closely related to the phenomenon involved in the future change. The validity of a distorted estuary model can only be assured for certain specialized phenomena which have been established through the verification process. Unfortunately there is a tendency to extend the usage of such models for predictive purposes beyond the scope of the physical processes used in the verification studies. This is especially true in the area of water quality investigations on physical models which were designed and verified for the study of navigation improvements.

The above remarks are not intended to discount the usage of physical models in certain water quality investigations. Rather it is a plea that the careful verification procedures used for the original purpose of the model be extended into the verification of flow phenomena which are uniquely associated with water quality problems.

2. SIMILITUDE OF MOMENTUM TRANSFER PROCESSES IN TIDAL MOTION

In this section the basic similitude conditions for the advective motion are developed from the principles of inspectional analysis. This results in the Froudian scale ratios for velocity, discharge, and time. In addition, boundary conditions and roughness relations for physical hydraulic models are discussed.

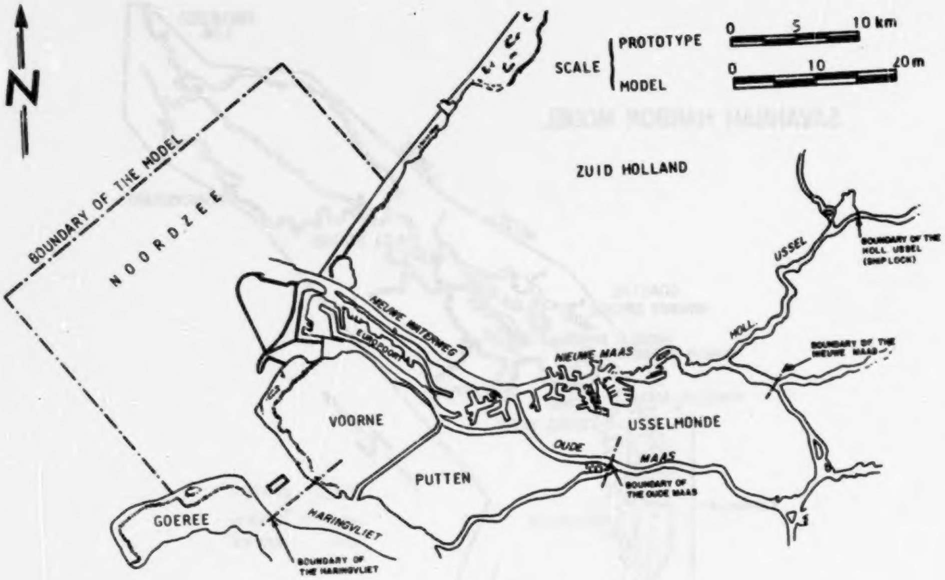
2.1 PHYSICAL BOUNDARY CONDITIONS FOR TIDAL MODELS

The first consideration in the design of a tidal model is the determination of the physical limits of the model. Usually an estuary model includes a portion of the ocean area in the form of a basin containing the ocean tide generator and provisions for maintaining a constant salinity representative of the ocean area. The shape and extent of the ocean basin depend on the complexity of tide and current conditions at the ocean entrance of the estuary. The tide generator may be required to produce sinusoidal tides with variable range, representing spring and neap conditions, or it may be designed to produce a complex mixed tide consisting of diurnal and semi-diurnal components.

Figure 5.1 shows the seaward boundaries of the model of the Rotterdam Waterway at the Delft Hydraulics Laboratory (Delft Hyd. Lab. 1969). The ocean basin has independent tide generators at the northeast and southwest boundaries of the basin representing the offshore area in the North Sea. In addition to the tidal oscillation, a current parallel to the coast may be produced. Vertical rotating cylinders have been used to simulate the deflection of the ebb flow from the estuary due to the rotation of the earth.

The landward extremity of a tidal model generally coincides with the upstream limit of tidal motion. In estuaries having a well-defined head of tide, such as a dam or natural fall, this location is readily determined. In some estuaries the tidal motion gradually diminishes in the upper reaches of tributary rivers. In this case the extent of tidal motion depends upon the ocean tide range and the magnitude of the freshwater inflow. In either case the landward boundary requires the reproduction of the temporal variation of freshwater inflows. Figure 5.2 shows the limits of the Delaware Estuary model which is typical of an estuary having a well-defined head of tide (at Trenton). The scale ratios are 1/1000 in the horizontal direction and 1/100 in the vertical direction. Figure 5.3 shows a similar view of the Savannah estuary model which is typical of the open-end type. The scale ratios are 1/800 horizontal and 1/80 vertical. Both models are of the fixed-bed type.

Where it is desirable to study only a limited portion of a tidal waterway, it is possible to terminate the model within the region of tidal motion. This requires the provision of a second, independently controlled tide generator at the inland boundary. This limits the use of the model since the inland tide generator can reproduce only those tidal stages and currents which have been observed in the prototype. If longitudinal salinity gradients due to salinity intrusion exist, it is usually not possible to terminate the model within this region because of the difficulty of controlling salinity variations at the inland boundary. Figure 5.4 shows the model limits of Absecon Inlet on the New Jersey coast. This model had a primary tide generator in the Atlantic ocean basin and a secondary generator at


N
SCALE
PROTOTYPE
0 5 10 km
MODEL
0 10 20 m
ZUID HOLLAND
BOUNDARY OF THE MODEL
NOORDZEE
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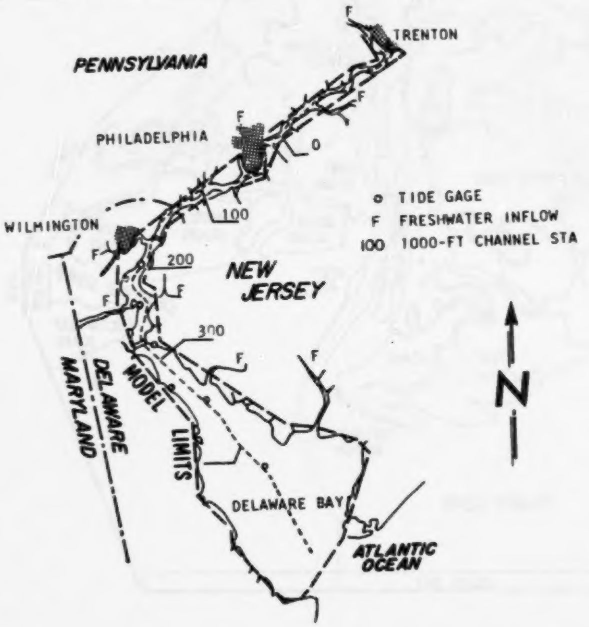
EUROPOORT
NIEUWE MAAS
USSEL
BOUNDARY OF THE HOLL. USSEL (SHIP LOCK)
HOLL.
BOUNDARY OF THE NIEUWE MAAS
VOORNE
USSELMONDE
OUDE
MAAS
PUTTEN
BOUNDARY OF THE OUDE MAAS
GOEREE
HARINGVLIET
BOUNDARY OF THE HARINGVLIET

Fig. 5.1 Model of the Rotterdam Waterway - Delft Hydraulics Laboratory (1969).


F
TRENTON
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F
200
NEW JERSEY
F
F
300
F
F
DELAWARE
MARYLAND
MODEL
LIMITS
DELAWARE BAY
ATLANTIC OCEAN
N

Fig. 5.2 Model of the Delaware Estuary - Waterways Experiment Station (1956).

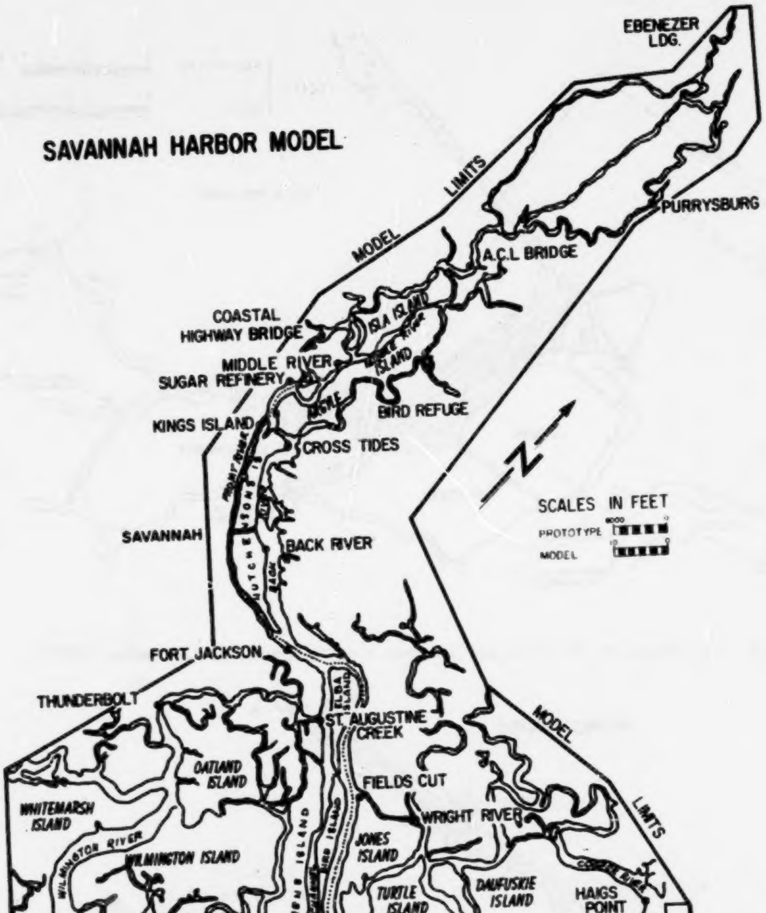
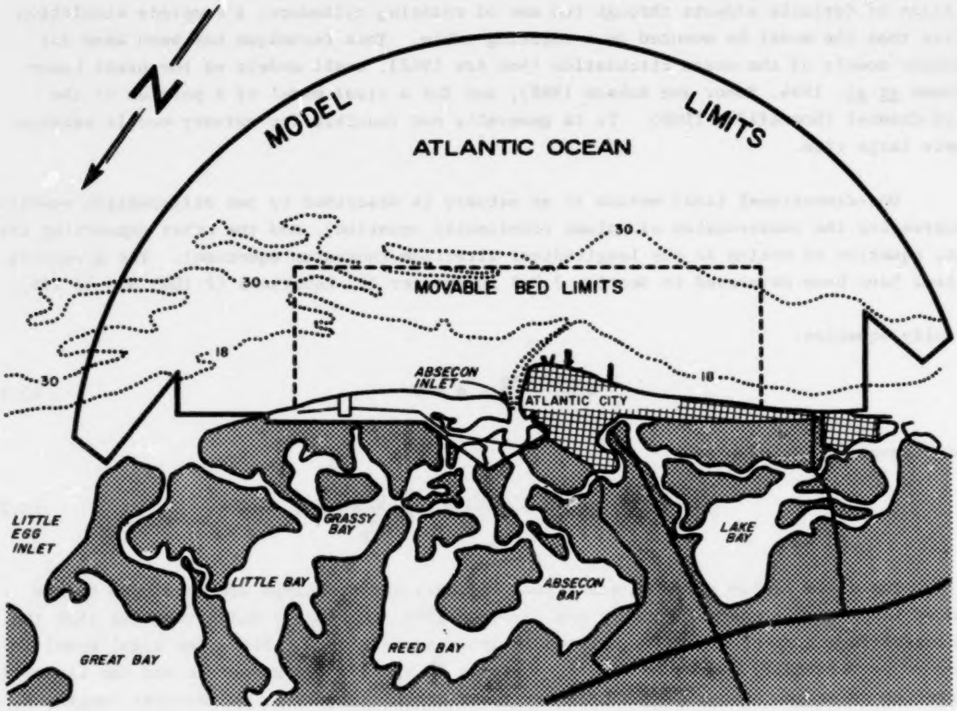

SAVANNAH HARBOR MODEL
EBENEZER LDG.
MODEL LIMITS
PURRYSBURG
A.C.L BRIDGE
COASTAL HIGHWAY BRIDGE
ISLA ISLAND
MIDDLE RIVER
SUGAR REFINERY
BIRD REFUGE
KINGS ISLAND
CROSS TIDES
SCALES IN FEET
PROTOTYPE
MODEL
SAVANNAH
BACK RIVER
FORT JACKSON
ELBA ISLAND
THUNDERBOLT
ST. AUGUSTINE CREEK
OATLAND ISLAND
FIELDS CUT
WHITEMARSH ISLAND
WRIGHT RIVER
WILMINGTON RIVER
WILMINGTON ISLAND
JONES ISLAND
TURTLE ISLAND
DAUFUSKIE ISLAND
HAIGS POINT
FORT PULASKI
HEAD BAY
CALIBOGUE SOUND
HILTON HEAD ISLAND
WASSAW SOUND
TYBEE ISLAND
SAVANNAH BEACH
ATLANTIC OCEAN
HEAD BAY

Fig. 5.3 Savannah Harbor Model - Waterways' Experiment Station


N
MODEL LIMITS
ATLANTIC OCEAN
30
30
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MOVABLE BED LIMITS
18
18
ABSECON INLET
ATLANTIC CITY
LITTLE EGG INLET
GRASSY BAY
LITTLE BAY
ABSECON BAY
LAKE BAY
REED BAY
GREAT BAY

Fig. 5.4 Absecon Inlet Model - Waterways Experiment Station.

the model limit in the inlet. In addition, surface waves were produced by a wave generator in the ocean basin. The scales were 1/500 horizontal and 1/100 vertical and the model had a moveable bed composed of fine sand.

2.2 FROUDE SCALE RATIOS FOR TIDAL MOTION

Tidal motion may be broadly classified into one-dimensional and two-dimensional categories. In the one-dimensional category, the lateral boundaries of the system constrain the tidal motion to a direction which roughly coincides with a centerline drawn between the adjacent boundaries. Tides in long, narrow gulfs or bays, fjords, estuaries and sea-level canals can generally be treated in the one-dimensional category. Two-dimensional considerations are generally necessary in treating tidal motion in broad bays, the mouths of certain estuaries on the continental shelf, wide straits, gulfs and enclosed seas. In these cases, the influence of the earth's rotation, through the Coriolis terms, must be considered. Aside from local simulation of Coriolis effects through the use of rotating cylinders, a complete simulation requires that the model be mounted on a rotating table. This technique has been used for hemisphere models of the ocean circulation (Von Arx 1962), small models of the Great Lakes (Harleman et al. 1964, Rumer and Robson 1968), and for a tidal model of a portion of the English Channel (Bonnefille 1969). It is generally not feasible for estuary models because of their large size.

One-dimensional tidal motion in an estuary is described by two differential equations, one expressing the conservation of volume (continuity equation), and the other expressing the dynamic equation of motion in the longitudinal direction (momentum equation). The governing equations have been developed in Section 3.2.3 in Chapter II, Equations (2.106) and (2.116).

Continuity equation:

$$b \frac{\partial h}{\partial t} + \frac{\partial Q}{\partial x} - q = 0 \qquad (5.1)$$

Momentum equation:

$$\frac{\partial Q}{\partial t} + U \frac{\partial Q}{\partial x} + Q \frac{\partial U}{\partial x} + g \frac{\partial h}{\partial x} A + g \frac{Q|Q|}{A C_h^2 R} = 0 \qquad (5.2)$$

The scale ratios relating quantities in model and prototype are developed by the method of inspectional analysis (Daily and Harleman 1966, Chapter 7) which requires that the governing differential equations be written in dimensionless form. Since the tidal model is assumed to be vertically distorted, it is necessary to specify two geometric and one kinematic parameter as reference quantities. These are a horizontal length L, a vertical length Y, and a reference velocity U_o. The following set of dimensionless variables (identified by a superscript o) are defined:

$$\begin{aligned} x^o &= x/L & t^o &= tU_o/L \\ b^o &= b/L & A^o &= A/LY \\ h^o &= h/Y & Q^o &= Q/LYU_o \\ U^o &= U/U_o & R^o &= R/Y \end{aligned} \qquad (5.3)$$

The dimensionless form of the continuity equation (5.1), obtained by substituting the above, is

$$b^o \frac{\partial h^o}{\partial t^o} + \frac{\partial Q^o}{\partial x^o} - q^o = 0 \qquad (5.4)$$

In a similar manner the dimensionless form of the momentum equation is obtained

$$\frac{\partial Q^o}{\partial t^o} + U^o \frac{\partial Q^o}{\partial x^o} + Q^o \frac{\partial U^o}{\partial x^o} + \left(\frac{1}{F^2}\right) \frac{\partial h^o}{\partial x^o} A^o + \left(\frac{gL}{C_h^2 Y}\right) \frac{Q^o|Q^o|}{A^o R^o} = 0 \qquad (5.5)$$

where $F = U_o / \sqrt{gY}$ is the Froude number.

The model and prototype will be dynamically similar if the two coefficients of Equation (5.5) are numerically the same in the two systems. Equality of the first coefficient is obtained by equating the Froude numbers

$$F_m = F_p \tag{5.6}$$

where the subscripts m and p refer to model and prototype. Equation (5.6) implies that

$$F_r \frac{U_r}{\sqrt{g_r Y_r}} = 1 \tag{5.7}$$

where the subscript r indicates the ratio of corresponding quantities in model and prototype. Since $g_r = 1$ the velocity ratio is given by

$$U_r = Y_r^{1/2} \tag{5.8}$$

and the discharge ratio is

$$Q_r = A_r U_r = L_r Y_r^{3/2} \tag{5.9}$$

The time ratio is

$$t_r = \frac{L_r}{U_r} = \frac{L_r}{Y_r^{1/2}} \tag{5.10}$$

Equality of the second coefficient in Equation (5.5) is given by

$$\left(\frac{gL}{C_h^2 Y}\right)_m = \left(\frac{gL}{C_h^2 Y}\right)_p \tag{5.11}$$

or

$$\frac{g_r L_r}{C_{h_r}^2 Y_r} = 1 \tag{5.12}$$

The Chezy coefficient can be expressed in terms of the Manning roughness n,

$$C_h = \frac{1.49}{n} R^{1/6} \tag{5.13}$$

or

$$C_{h_r} = \frac{R_r^{1/6}}{n_r} \tag{5.14}$$

In a wide, shallow channel the hydraulic radius is essentially equal to the depth, therefore, with $R_r = Y_r$ and combining Equations (5.12) and (5.14),

$$n_r = \frac{Y_r^{2/3}}{L_r^{1/2}} \tag{5.15}$$

In a typical model in which $L_r = 1/1000$ and $Y_r = 1/100$, the velocity ratio $U_r = 1/10$, the discharge ratio $Q_r = 1/10^6$, the time ratio $t_r = 1/100$ and the roughness ratio $n_r = 1.46$. The latter indicates that the model roughness should be approximately 50 percent greater than the prototype.

The scale ratios for velocity, discharge and time which are derived from the Froude number equality should be strictly maintained, however the roughness indicated by Equation (5.15) should be regarded as a first approximation. It will be necessary to adjust the model roughness during the verification phase. This is due to the following factors: (i) uncertainty in the magnitude of the prototype roughness and its spatial distribution; (ii) the assumption of hydraulically rough flow in the model is not correct since there will be periods of non-turbulent flow near the times of slack tide; (iii) the assumption that the hydraulic radius is equal to the depth is not correct in the distorted section of the model. The form of the model roughness elements which are used to achieve the high degree of resistance indicated by Equation (5.15) is an important factor. The required energy dissipation can be obtained by blocks or stones attached to the model bottom, or by vertical rods or strips extending almost the full water depth. The choice of resistance elements will be discussed in a later section. In this connection it will be helpful to determine the ratio of the rates of energy dissipation per unit mass of fluid in model and prototype. The rate of energy dissipation is given by $\gamma Q S_E \Delta x$, where γ is the specific weight, Q the discharge and S_E the slope of the energy gradient. The mass of fluid is given by $\rho A \Delta x$ where ρ is the density and A the cross-sectional area. The rate of energy dissipation per unit mass of fluid, G, is given by

$$G = g \frac{QS_E}{A} \tag{5.16}$$

and the model-prototype ratio is

$$G_r = g_r \frac{Q_r (S_E)_r}{A_r} = g_r \, U_r (S_E)_r$$

The scale ratio for the slope of the energy gradient $(S_E)_r = Y_r/L_r$ and U_r is given by Equation (5.8), therefore

$$G_r = \frac{Y_r^{3/2}}{L_r} \tag{5.17}$$

For the frequently used scales of $L_r = 1/1000$ and $Y_r = 1/100$, the magnitude of G_r is unity. Thus, in a distorted model having these scale ratios, the rates of energy dissipation per unit mass of fluid in model and prototype are equal.

The scale ratios derived in this section provide all the necessary relations for the control of tidal motion in the model. For example, if the prototype has a semi-diurnal tidal period of 12.4 hours, the tidal period of a distorted model having $L_r = 1/1000$ and $Y_r = 1/100$ as given by Equation (5.10) is 7.5 minutes. The tidal range in the ocean basin is scaled from prototype range in accordance with the vertical scale ratio Y_r. Tidal velocities in model and prototype are related by the velocity ratio given by Equation (5.8) and freshwater tributary discharges are related by Equation (5.9).

2.3 REYNOLDS NUMBER EFFECTS

The foregoing development contains no similitude condition involving the fluid viscosity or its associated dimensionless parameter known as the Reynolds number. This is due to the fact that the quadratic friction term characteristic of hydraulically rough turbulent flow was included in the longitudinal momentum Equation (5.2). The quadratic assumption is justified for the prototype, and in view of the high roughness distortion it is a reasonable assumption for the model provided the flow is predominantly in the turbulent regime. When the same fluids are used in model and prototype it is impossible to have equality of both Froude and Reynolds numbers. Therefore it must be accepted that the Reynolds number of the model will always be considerably less than that of the prototype. The Reynolds number ratio is given by

$$\mathcal{R}_r = \frac{U_r Y_r}{\nu_r} \qquad (5.18)$$

The velocity ratio must satisfy the Froude similitude condition of Equation (5.8) and since $\nu_r = 1$,

$$\mathcal{R}_r = Y_r^{3/2} \qquad (5.19)$$

If $Y_r = 1/100$, the model Reynolds number will be 1/1000 of the prototype.

3. SIMILITUDE OF MASS TRANSFER PROCESSES

In this section the basic similitude conditions for mass transfer processes are developed from the principles of inspectional analysis (Harleman et al. 1966). The similitude of mass transfer implies that the concentration of a certain substance measured in the model at a fixed point and time is identically equal to the concentration in the prototype at a geometrically similar point and kinematically similar time. In an estuary model, where geometric distortion is always a necessity, the geometrically similar points are related by the horizontal and vertical scale ratios. Since the advective processes (tidal motion and freshwater inflow) must satisfy the Froude relationships developed in Section 2, the model-prototype times are related to the geometric scales by Equation (5.10). If the mass transfer similitude conditions can be satisfied, in addition to the Froude conditions required by the advective processes, the scale ratio for concentrations should be unity since concentration is a dimensionless quantity (mass or volume of substance per unit mass or volume of solution). This statement implies that all boundary conditions relating both to the advective processes and to the introduction of the substance into the estuary are correctly reproduced in the physical hydraulic model.

To determine the conditions under which mass transfer similitude can be achieved, it is necessary to postulate the form of the differential equation governing the mass transfer process. In water quality applications we are generally concerned with the distribution and effect of one or more effluents discharged into an estuary or tidal waterway. If the effluent is discharged into the salinity intrusion region, the mass transfer will depend on whether the estuary is stratified or mixed. The governing equations in the two cases are quite different and the correct reproduction of the salinity intrusion process will be an essential feature of the physical model. If the effluent is discharged into a tidal region consisting of entirely fresh or homogeneous saline water, the correct reproduction of concentration distribution will depend on the ability of the reduced scale model to simulate dispersion associated with the tidal advection.

3.1 SIMILITUDE OF SALINITY INTRUSION

The majority of existing estuary models were originally constructed for the purpose of studying shoaling processes. It is well known that the intrusion of saline water is a major factor in the distribution of sediment in estuaries (Wicker and Eaton 1965, Ippen 1966b and 1966c, Harleman and Ippen 1969). In hydraulic model practice the reproduction of salinity intrusion in both the horizontal and vertical dimensions has been largely a result of empirical adjustments during the second stage of model verification. The first stage of model verification is concerned with the tidal motion and involves the reproduction of local tidal range, phase, current distribution and magnitude. These are based on the Froude scale ratios derived in the previous section and verification is obtained by local adjustment and distribution of roughness elements. Experience has shown that the form of the resistance elements should be chosen in relation to the type of salinity intrusion which is to be reproduced. The salinity intrusion can be broadly grouped into two categories: the saline wedge and the mixed estuary. In Pritchard's (1955) classification these correspond to type A and B respectively. Harleman and Abraham (1966) suggest the use of a dimensionless estuary number as a means of classifying estuaries in terms of vertical mixing. The estuary number is defined in the following manner:

$$\text{estuary number} = \frac{P_t F_o^2}{Q_f T} \qquad (5.20)$$

where P_t = tidal prism or volume of sea water entering the estuary on the flood tide

$F_o = U_o/\sqrt{gh}$, where U_o is the maximum tidal velocity at the estuary mouth and h is the mean depth

Q_f = freshwater inflow rate

T = tidal period

Estuaries of the saline-wedge type appear to have values of this parameter smaller than 0.001, whereas the value approaches unity for the highly mixed types. This suggests that the saline wedge occurs with a combination of small tidal range (small P_t and F_o) and large freshwater discharge. There are relatively few classical saline-wedge estuaries in the United States. One of the best examples is the mouth of the Mississippi where the freshwater flow almost completely dominates the circulation. Profiles of the salt water interface for various rates of freshwater flow in the Mississippi River are shown in Figure 5.5.

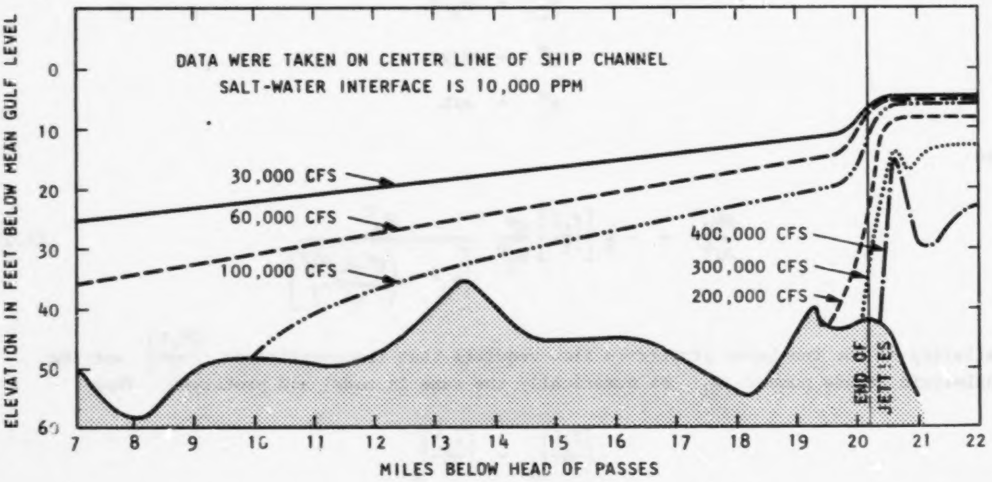


Fig. 5.5 Profiles of salt-water interface at mouth of Mississippi for various freshwater discharges. After Rhodes (1950).

3.1.1 Saline-Wedge Estuary

The salinity and velocity distributions in a saline-wedge estuary are shown schematically in Figure 5.6. A summary of experimental and analytical investigations on this type of estuary has been given by Keulegan (1966). An equation for the slope of the interface in a general two-layer stratified flow can be developed by writing the one-dimensional equations of motion and continuity for both the upper (fresh water) and lower (salt water) layers (Schijf and Schonfeld 1953, Harleman 1960 and 1969). For the special case of an arrested saline wedge in which the mean velocity of the salt water layer is zero, the differential equation for the slope of the interface has the following form:

$$\frac{dh_2}{dx} = -\frac{f_i}{8}\frac{H}{H_2}\frac{F_H^{\,2}}{\left[F_H^{\,2} - \left(\frac{H-h_2}{H}\right)^3\right]} \qquad (5.21)$$

where f_i is the mean friction coefficient for the interfacial shear stress and the other quantities are as defined in Figure 5.7. F_H is the densimetric Froude number given by

$$F_H = \frac{U_H}{\sqrt{g\,\frac{\Delta\rho}{\rho}\,H}} \qquad (5.22)$$

Equation (5.21) can be written in dimensionless form by defining characteristic horizontal and vertical lengths L and Y, such that

$$h_2^{\,o} = h_2/Y$$

$$H^o = H/Y$$

$$x^o = x/L$$

then

$$\frac{dh_2^{\,o}}{dx^o} = -\frac{1}{8}\left[\frac{f_i L}{Y}\right]\frac{H^o}{h_2^{\,o}}\frac{F_H^{\,2}}{\left[F_H^{\,2} - \left(\frac{H^o-h_2^{\,o}}{H^o}\right)^3\right]} \qquad (5.23)$$

Similarity of the two-layer stratified flow requires that the coefficient $\left[\frac{f_i L}{Y}\right]$ and the densimetric Froude number F_H be numerically the same in model and prototype. Thus

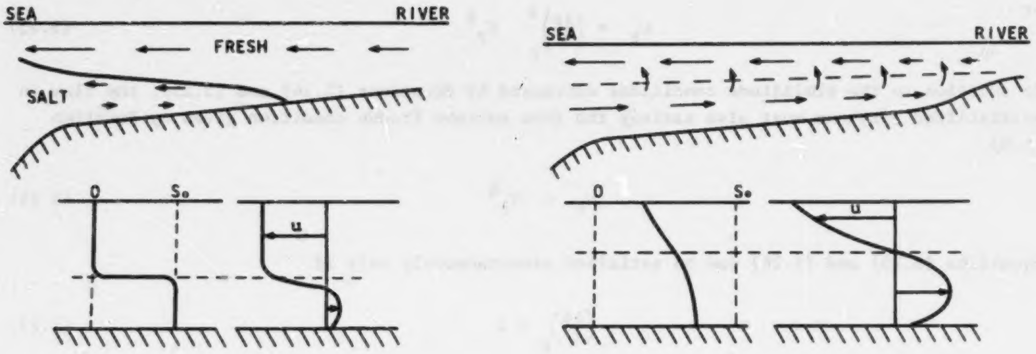
$$\left[\frac{f_i L}{Y}\right]_m = \left[\frac{f_i L}{Y}\right]_p$$

or

$$(f_i)_r = Y_r/L_r \qquad (5.24)$$

and

$$[F_H]_m = [F_H]_p$$


SEA
RIVER
FRESH
SALT
O
S₀
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SEA
RIVER
O
S₀
u

Salt wedge estuary: Above - section along estuary; Below - typical salinity and velocity profiles.

Partially mixed estuary with entrainment and mixing: Above - section along estuary; Below - typical salinity and velocity profiles.

Fig. 5.6 Circulation in salt wedge and partially mixed estuaries.

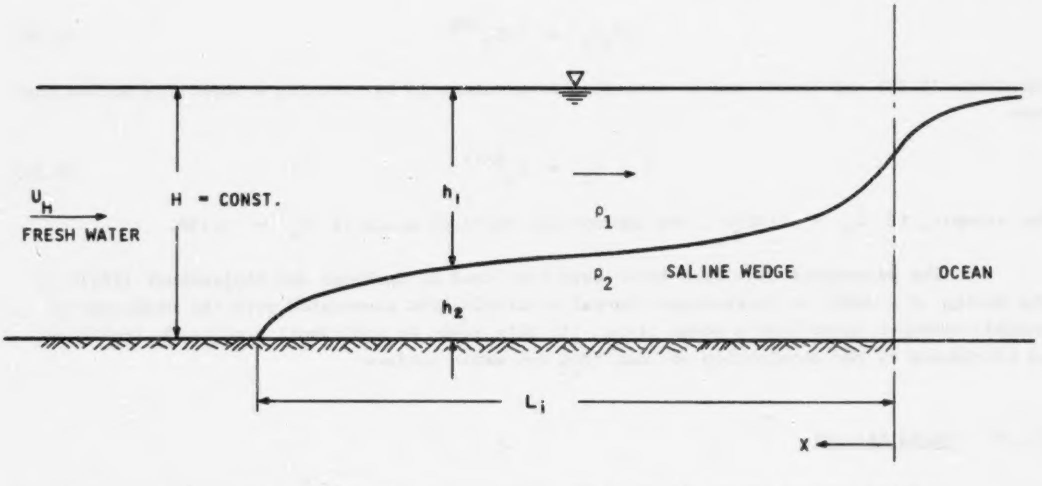

U_H
FRESH WATER
H = CONST.
h_1
ρ_1
ρ_2
SALINE WEDGE
OCEAN
h_2
L_i
X

Fig. 5.7 Arrested saline wedge near the ocean entrance of a freshwater channel.

or

$$U_r = \left(\frac{\Delta\rho}{\rho}\right)_r^{\frac{1}{2}} \; Y_r^{\frac{1}{2}} \tag{5.25}$$

In addition to the similitude conditions expressed by Equations (5.24) and (5.25), the flow in unstratified portions must also satisfy the free surface Froude condition given by Equation (5.8),

$$U_r = Y_r^{\frac{1}{2}} \tag{5.26}$$

Equations (5.25) and (5.26) can be satisfied simultaneously only if

$$\left(\frac{\Delta\rho}{\rho}\right)_r = 1 \tag{5.27}$$

which implies that the density differences in model and prototype must be identical.

To satisfy the similitude requirement of Equation (5.24), an assumption as to the nature of the interfacial shear stress in both model and prototype must be made. One possible assumption is that both follow the smooth-turbulent resistance law in the form of the Blasius equation

$$f_i = \frac{0.316}{\mathcal{R}^{\frac{1}{4}}} \tag{5.28}$$

where $\mathcal{R}$ is a Reynolds number characteristic of the flow. From Equation (5.28) we find

$$(f_i)_r = 1/\,\mathcal{R}_r^{1/4} \tag{5.29}$$

and since $\mathcal{R}_r = Y_r^{3/2}$ (Equation 5.19)

$$(f_i)_r = 1/Y_r^{3/8} \tag{5.30}$$

Equations (5.24) and (5.29) can be satisfied simultaneously by choosing a model distortion such that

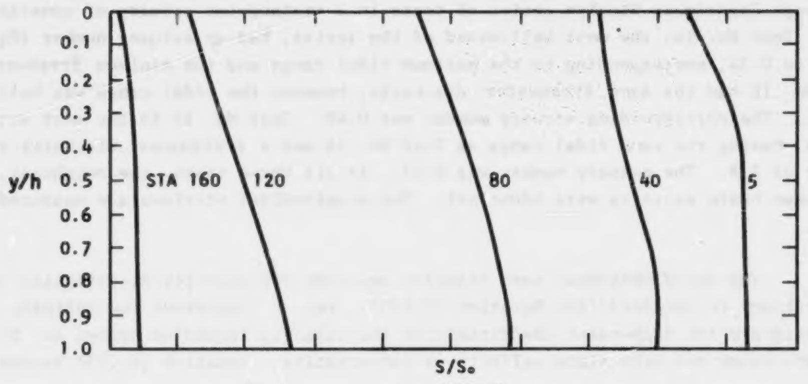
$$Y_r = L_r^{8/11} \tag{5.31}$$

For example, if $L_r = 1/1000$, the appropriate vertical scale is $Y_r = 1/150$.

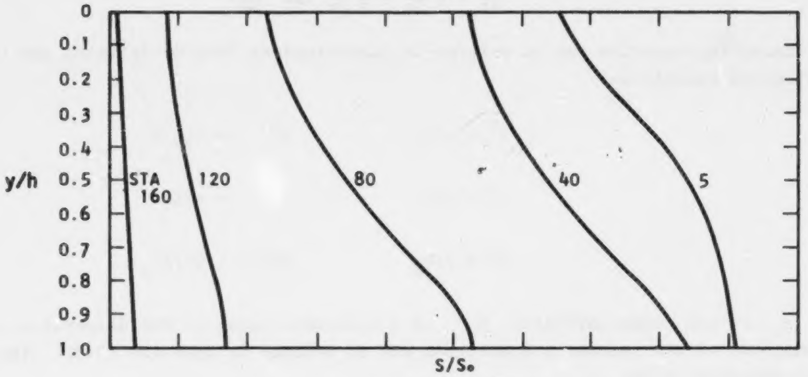
The procedures developed above have been used by Harleman and Stolzenback (1967) in the design of a model to investigate thermal stratification associated with the discharge of heated condenser water from a power plant. In this study an additional similitude requirement is introduced by the dissipation of heat from the water surface.

3.1.2. Mixed Estuary

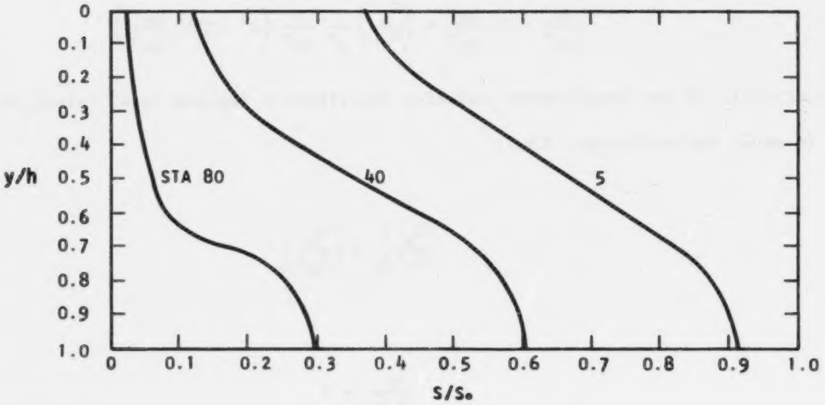
A mixed estuary is one in which the tidal motion is sufficient to induce vertical mixing in spite of the stabilizing influence of the vertical density distribution. The majority of United States estuaries are classified as mixed estuaries with varying degrees of vertical mixing. The range of mixed types is illustrated in Figure 5.8 showing laboratory data from the



a. TEST 14



b. TEST 16



c. TEST 11

Fig. 5.8 Horizontal and vertical salinity distributions characteristic of well-mixed (a) and partially-mixed estuaries (c).

Waterways Experiment Station series of tests in a rectangular estuary of constant cross-sectional area. Test No. 14, the most well-mixed of the series, had an estuary number (Equation 5.20) equal to 0.34, corresponding to the maximum tidal range and the minimum freshwater inflow. Test No. 16 had the same freshwater discharge, however the tidal range was half that of Test No. 14. The corresponding estuary number was 0.08. Test No. 11 is the most stratified of the series, having the same tidal range as Test No. 16 and a freshwater discharge increase by a factor of 2.8. The estuary number was 0.03. In all three tests, the roughness, mean depth and ocean basin salinity were identical. The longitudinal stations are measured from the ocean basin.

The one-dimensional mass transfer equation for salinity distribution in a variable-area estuary is obtained from Equation (2.133). Let s represent the salinity concentration and designate the dispersion coefficient in the salinity intrusion region as E'. The source and sink terms are zero since salinity is conservative. Equation (2.133) becomes

$$\frac{\partial s}{\partial t} + U \frac{\partial s}{\partial x} = \frac{1}{A} \frac{\partial}{\partial x} \left(AE' \frac{\partial s}{\partial x}\right) \tag{5.32}$$

The differential equation can be written in dimensionless form by defining the following dimensionless quantities:

$$\begin{array}{ll} s^o = s/s_o & t^o = tU_o/L \\ x^o = x/L & A^o = A/LY \\ U^o = U/U_o & (E')^o = E'/E'_o \end{array} \tag{5.33}$$

where s_o is the ocean salinity, E_o' is a reference value of the dispersion coefficient and the remainder of the reference quantities are as defined in Equation (5.3). The dimensionless form of Equation (5.32) is

$$\frac{\partial s^o}{\partial t^o} + U^o \frac{\partial s^o}{\partial x^o} = \left(\frac{E_o'}{U_o L}\right) \frac{1}{A^o} \frac{\partial}{\partial x^o} \left(A^o \, (E')^o \, \frac{\partial s^o}{\partial x^o}\right) \tag{5.34}$$

and similarity of the longitudinal salinity distribution implies equal values of the coefficient $\frac{E_o'}{U_o L}$ in model and prototype. Thus,

$$\left(\frac{E_o'}{U_o L}\right)_m = \left(\frac{E_o'}{U_o L}\right)_p$$

or

$$\frac{E_r'}{U_r L_r} = 1 \tag{5.35}$$

The advective process must satisfy the Froude similitude condition, therefore $U_r = Y_r^{1/2}$ (Equation 5.8) and

$$E_r' = Y_r^{1/2} L_r \tag{5.36}$$

In a typical estuary model in which $L_r = 1/1000$ and $Y_r = 1/100$, the ratio of dispersion coefficients in the salinity intrusion region is

$$E_r' = 1/10{,}000$$

In hydraulic models of mixed estuaries, there has been a fairly high degree of success in reporducing the salinity distributions observed in the prototype during the model verification process. In practice, the fresh-ocean water density difference has usually been equal in model and prototype, although there is no strict necessity for density equality in models of mixed estuaries.

3.2 MASS TRANSFER SIMILITUDE IN REGIONS OF UNIFORM DENSITY

We consider an effluent discharging into a tidal region consisting of fresh water or homogeneous saline water in which the effluent substance is undergoing a first-order decay. In the absence of longitudinal and vertical salinity gradients, the dispersion is related to the tidal advection (through the depth and shear velocity) by the Taylor-Elder dispersion equation (2.124). The differential equation for the mass transfer process, Equation (2.133), with $r_e = 0$ and $r_i/\rho = -K_d C$, is

$$\frac{\partial C}{\partial t} + U \frac{\partial C}{\partial x} = \frac{1}{A} \frac{\partial}{\partial x} \left(A E_L \frac{\partial C}{\partial x} \right) - K_d C \tag{5.37}$$

With the reference quantities L, Y, C_o, U_o and E_o, the dimensionless form of Equation (5.37) becomes

$$\frac{\partial C^o}{\partial t^o} + U^o \frac{\partial C^o}{\partial x^o} = \left(\frac{E_o}{U_o L} \right) \frac{1}{A^o} \frac{\partial}{\partial x^o} \left(A^o E_L{}^o \frac{\partial C^o}{\partial x^o} \right) - \left(\frac{K_d L}{U_o} \right) C^o \tag{5.38}$$

Concentration distributions in model and prototype will be similar only if the two coefficients of Equation (5.38) are numerically equal in the two systems. Equality of the first coefficient requires that

$$\frac{E_r}{U_r L_r} = 1 \tag{5.39}$$

or, since $U_r = Y_r^{1/2}$,

$$E_r = L_r Y_r^{1/2} \tag{5.40}$$

In a uniform-density tidal region, the ratio of model and prototype dispersion is given by the Taylor-Elder equation (2.124), thus

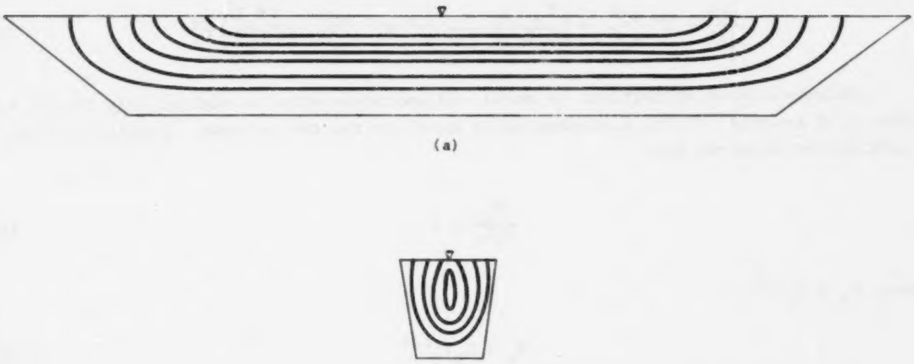
$$E_r = d_r \sqrt{g_r d_r (S_E)_r} \tag{5.41}$$

The depth ratio $d_r = Y_r$, $g_r = 1$ and the ratio of energy gradient slope in a distorted model is $(S_E)_r = Y_r/L_r$. Therefore Equation (5.41) becomes

$$E_r = Y_r^{2}/L_r^{1/2} \tag{5.42}$$

(Harleman et al. 1966).

It is apparent that there is a direct conflict between the similitude requirement for the ratio of dispersion coefficients as expressed by Equation (5.40) and the ratio of dispersion coefficients predicted from fluid mechanics considerations as expressed by Equation (5.42). It should be noted that this conflict does not arise in the salinity intrusion region, provided that the hydraulic model is made to agree with the prototype through the process of verification of the salinity distribution. In a distorted model with $L_r = 1/1000$ and $Y_r = 1/100$, the ratio of dispersion coefficients required by Equation (5.40) is 1/10,000 , whereas the predicted dispersion coefficient ratio is 1/316. This means that the dispersion coefficient in the uniform-density tidal region of a distorted hydraulic model is much too large. For the above horizontal and vertical scale ratios, the dispersion coefficient is too large by a factor of approximately 30. The physical explanation of dispersion, as given in Section 3.2.4 of Chapter II, points out that the magnitude of the dispersion coefficient is governed by the nonuniformity of the velocity distribution. Figure 5.9(a) shows a schematic velocity distribution in a wide, shallow estuary cross section and Figure 5.9(b) shows the same section with a distortion ratio of 10. It is apparent that the velocity distribution in the distorted section is relatively much more nonuniform than in the wide, shallow section; therefore, the dispersion is distorted.



(a)

(b)

Fig. 5.9 Comparison of velocity distributions in channels having a 10 to 1 distortion.

Quantitative results substantiating the above conclusion are given in the following manner:

(i) Assume that, because of verification, the dispersion coefficients in the salinity intrusion region in model and prototype are in accord with the similitude requirement given by Equation (5.36). It follows that

$$E_m' = E_p' \, Y_r^{1/2} \, L_r \qquad (5.43)$$

(ii) Assume that the ratio of dispersion coefficients in model and prototype in the uniform-density tidal region are in accord with the Taylor relation given by Equation (5.42). It follows that

$$E_m = E_p \, Y_r^{2}/L_r^{1/2} \qquad (5.44)$$

The division of Equation (5.43) by Equation (5.44) results in an expression for the relative magnitude of dispersion coefficients in the salinity intrusion and uniform-density regions in model and prototype,

$$\frac{E_m'}{E_m} = \frac{E_p'}{E_p}\left(\frac{L_r}{Y_r}\right)^{3/2} \qquad (5.45)$$

(iii) The magnitudes of E_p' and E_p for the Rotterdam Waterway, as given in Section 3.2.4.2 of Chapter II, are $E_p' = 13{,}000$ ft^2/sec and $E_p = 175$ ft^2/sec. Thus the prototype ratio of

$$\frac{E_p'}{E_p} = 75$$

indicates a very large increase in dispersion due to the large-scale advective circulation induced by salinity gradients.

(iv) A series of salinity intrusion tests conducted in a model estuary at the Waterways Experiment Station was analyzed by Ippen and Harleman (1961, see also Ippen 1966a). The salinity in the model tidal basin varied between 5 ppt and 30 ppt (ocean salinity) in various tests, and for each test the magnitude of E_m' was determined. In addition, tests for each tidal condition were made in which the ocean basin contained fresh water with a dye tracer. These tests established the magnitude of the uniform-density dispersion coefficient E_m. The ratio E_m'/E_m is plotted in Figure 5.10 against a modification of the estuary number, Equation (5.20), defining the degree of vertical mixing. For the model tests in which the basin salinity was equal to 30 ppt, the increase in the dispersion coefficient due to salinity circulation is of the order of 4. Harleman and Abraham (1966) have pointed out that some of the W.E.S. salinity tests may be interpreted as models of the Rotterdam Waterway having a distortion $L_r/Y_r = 1/10$.

(v) The above data may be used to check the validity of Equation (5.45). If $E_p'/E_p = 75$ and $L_r/Y_r = 1/10$, the calculated value of $E_m'/E_m = 2.5$. This ratio compares favorably with the results given in Figure 5.10. It is concluded that the increase in dispersion due to salinity in the model is small because the dispersion in the uniform-density region has been magnified by the distortion of the geometry.

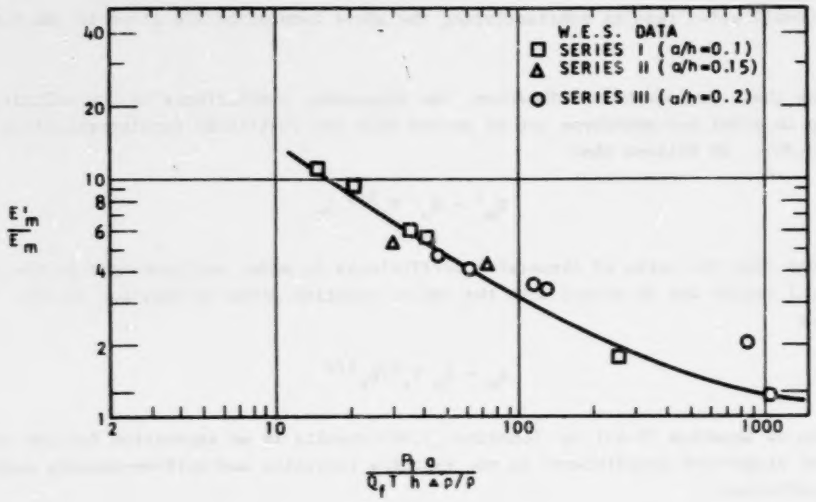


Fig. 5.10 **Ratio of dispersion coefficients with and without salinity induced circulation in a distorted tidal model at the Waterways Experiment Station.**

We return to Equation (5.38) to consider the second requirement for similarity which involves the decay rate constant. The equality of the second coefficient in Equation (5.38) is given by

$$\left(\frac{K_d L}{U_o}\right)_m = \left(\frac{K_d L}{U_o}\right)_p \tag{5.46}$$

or

$$\frac{(K_d)_r L_r}{U_r} = 1 \tag{5.47}$$

and since $U_r = Y_r^{1/2}$, it follows that

$$(K_d)_r = Y_r^{1/2}/L_r \tag{5.48}$$

Equation (5.48) could have been established independently by noting that the decay constant K_d has the dimensions of t^{-1} , therefore the ratio $(K_d)_r$ is the inverse of the time ratio given by Equation (5.10). In a distorted model in which $L_r = 1/1000$ and $Y_r = 1/100$, the ratio $(K_d)_r = 100$. Thus the decay constant for a substance introduced into the model should be one hundred times the prototype decay constant. The possibility of finding a model tracer substance satisfying this requirement is remote since the commonly used dyes such as Rhodamine have small decay rates which depend in part on the absorption of the dye on the boundary surfaces of the model. Thus, if tracer dyes are used in physical hydraulic models, the observed concentrations in the model must be corrected to equivalent concentrations for a

conservative substance by multiplying the observed concentrations by $e^{K_d t}$, where t is measured from the start of the dye injection. The determination of the appropriate value of K_d for the model is in itself a difficult task. It must be accomplished by periodically integrating the total mass of dye remaining in the fluid portions of the model and comparing this mass with the known quantity introduced.

4. MODEL VERIFICATION

Model verification is a process by which a hydraulic model is tested to determine its ability to reproduce certain phenomena which have been observed in the prototype. Whenever possible the model is adjusted by trial until reasonable agreement with field observations is obtained. The need for verification is due to the fact that the only precise scale ratios for a distorted model are those for velocity, discharge and time. Flow processes involving mixing, diffusion and dispersion are influenced by the geometric distortion of the cross section and its effect on velocity distributions, the low Reynolds number of the model in comparison with the prototype, and the arbitrary form and distribution of model roughness and mixing elements. The validity of model observations is strongly dependent on there being a close relationship between the phenomena observed in the model and the prototype phenomena used in the verification processes. For example, because of the marked difference in the mechanism of dispersion in salinity-gradient regions and in uniform-density tidal regions, the verification of salinity distributions in the model is no guarantee that dispersion in the uniform-density region is correctly reproduced in the model.

Model verification is a painstaking and time consuming process which may occupy a period of one or more years in a major estuary model. Adequate model verification requires the collection of extensive field data over a significant prototype time span. Very little general information has been published on verification techniques. They are highly dependent on the experience of the model operator and it is difficult to formulate general rules. Summary descriptions of some American tidal models and their verification have been prepared by Simmons (1966) and Simmons and Lindner (1965). The following sections illustrate model verification by showing comparisons of model-prototype data in certain studies.

4.1 TIDAL VERIFICATION

The first phase of model verification consists of checking the reproduction of all aspects of the tidal motion. This includes local water surface elevations, local time phase of tidal motion, and the vertical and lateral distribution of tidal currents. Adjustments are made in the model roughness which may consist of stones or rough stucco on the model bed in shallow portions. In deeper portions, vertical strips of thin metal (3/4" in width) extending to the low water elevation are commonly used. During the verification process, the strips, which are placed at the time of construction, may be cut, bent down or twisted to achieve the desired local effects.

Figure 5.11 shows a comparison of model and prototype data for the Delaware estuary (WES 1956) for tidal range, mean tide level and phase. The verification of tidal velocities is a much more difficult task. For one reason, it is known that the salinity intrusion has a marked effect on the distribution of tidal velocities. Therefore, it is usually necessary to maintain the ocean basin salinity and to introduce freshwater inflows, corresponding to conditions under which the prototype velocity measurements were made, prior to undertaking tidal velocity verification. The complexity of tidal velocity and salinity interaction can be seen by referring to field data for a section of the Savannah estuary near the mouth (Sta. 190) (Rhodes 1950). Figure 5.12 shows the temporal variation of salinity, tide height and current velocity for one tidal cycle at three different depths for a freshwater inflow of the order of

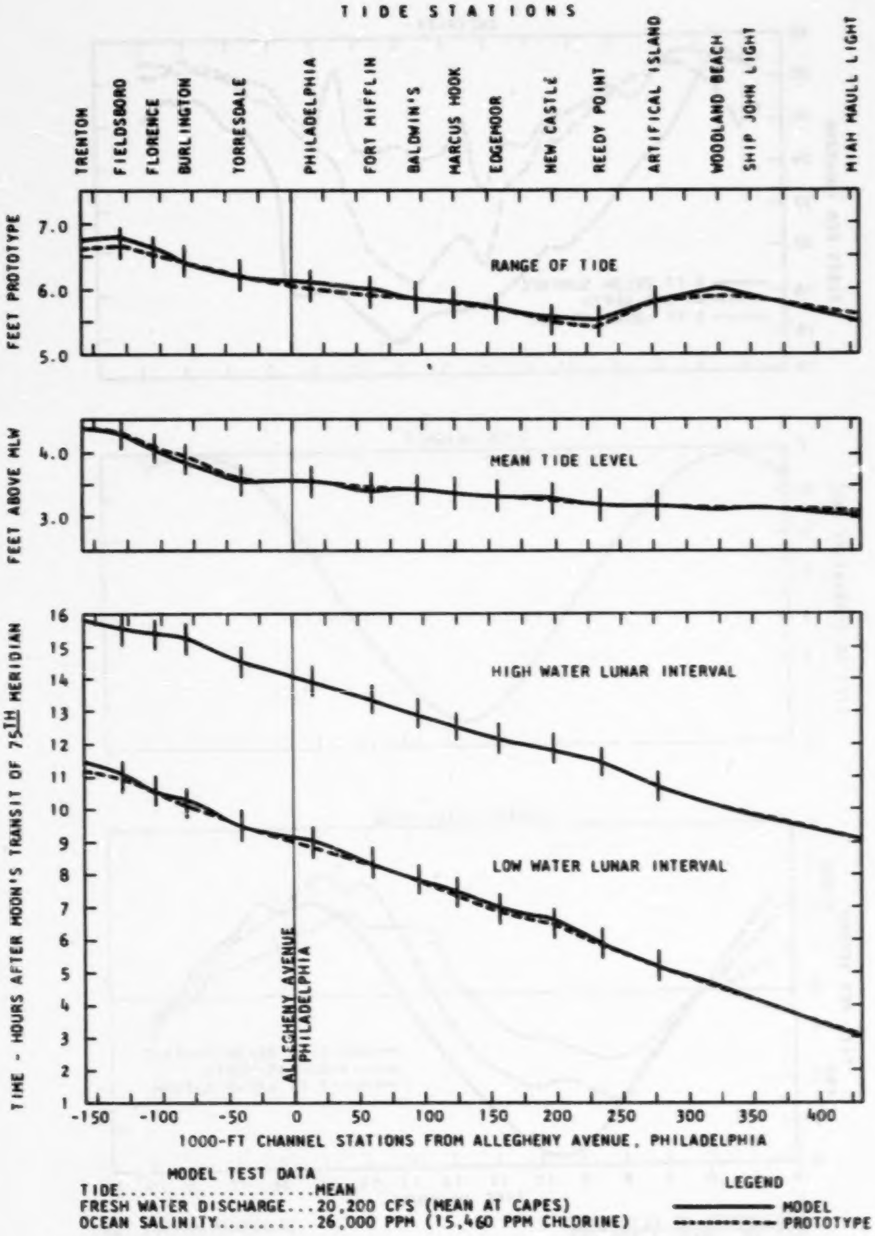
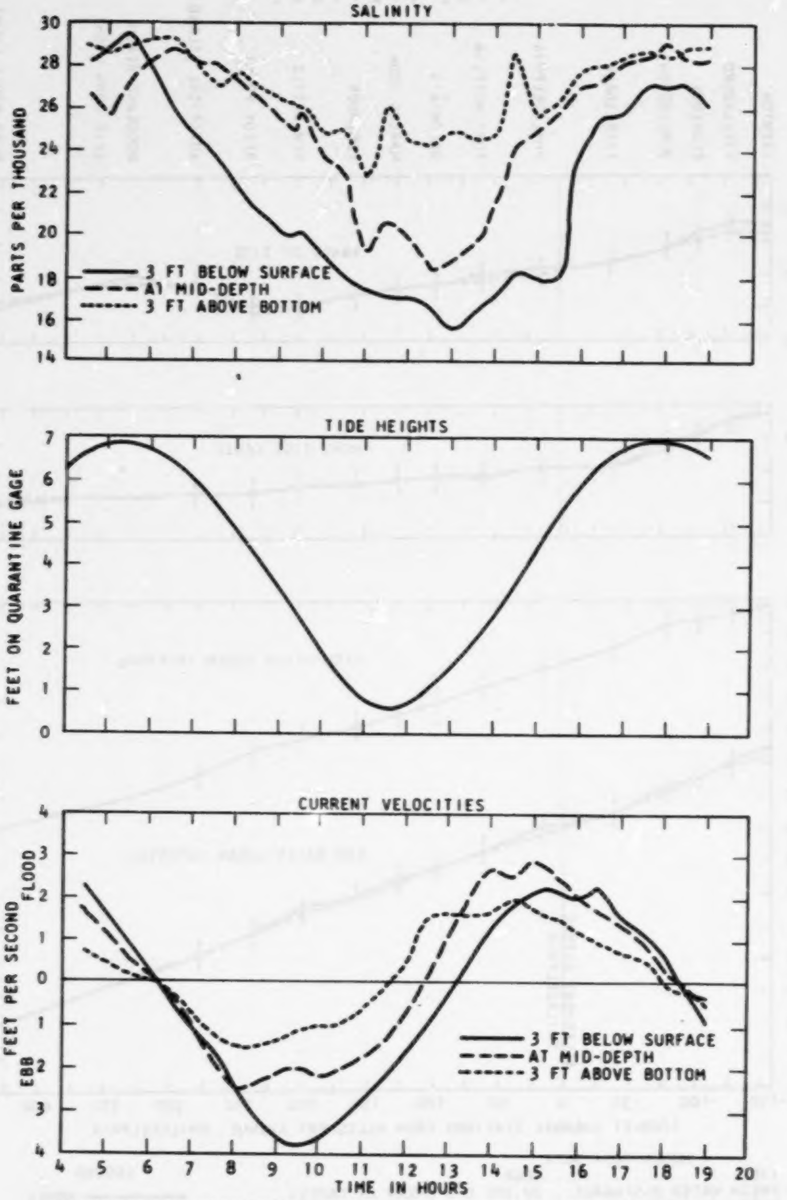


Fig. 5.11 Model-prototype verification for tidal range and phase - Delaware Estuary Model.



DISCHARGES AT CLYO GAGE
OCT 18, 1935, 3,700 CFS
OCT 19, 1935, 3,400 CFS
OCT 20, 1935, 3,300 CFS
OCT 21, 1935, 3,600 CFS
OCT 23, 1935, 3,800 CFS

SAVANNAH HARBOR, GA.
CURRENT - SALINITY DATA
STATION 190
23 OCTOBER 1935

Fig. 5.12 Vertical distribution of salinity and tidal current - Savannah Harbor. $Q_f = 3,800$ cfs. After Rhodes (1950).

3600 cfs. The data for the same station given in Figure 5.13, for an inflow of approximately 70,000 cfs, shows a marked change in both salinity and velocity. Figures 5.12 and 5.13 refer only to changes with depth at a fixed location. In addition, there are lateral variations as shown in Figure 5.14 at Station 155 in the Savannah estuary.

In the Delaware estuary, prototype velocity data for model verification were available at 74 locations. In about one-half of the locations velocities were measured at three different depths, while in the remainder only mid-depth values were available. Two velocity verification results are shown for the Delaware model. Figure 5.15 was selected as representatime of the better verifications, and Figure 5.16 is representative of the poorer verifications. In the latter case the maximum flood velocity near the bottom was 2.1 ft/sec in the prototype and 3.3 ft/sec in the model, or a difference of approximately 50%. The velocity verification consisted of local rearrangements of resistance elements with an attempt to keep the total resistance changes to a minimum. This is necessary because major changes would alter the local tidal elevation and phase which had been adjusted previously.

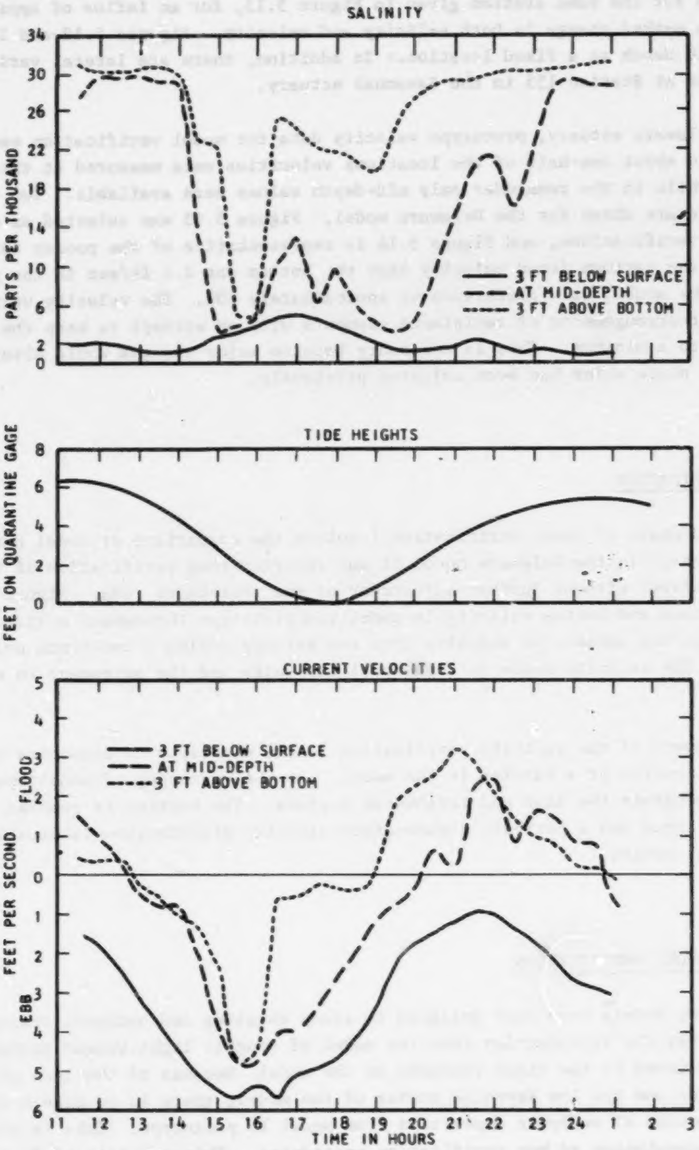
4.2 SALINITY VERIFICATION

The second phase of model verification involves the comparison of model and prototype salinity distributions. In the Delaware model it was reported that verification of the salinity distribution was achieved without further adjustment of the resistance rods. Figure 5.17 shows a comparison of surface and bottom salinity in model and prototype throughout a tidal cycle, and Figure 5.18 shows the advance of salinity into the estuary during a two-month period of low freshwater inflow. The salinity scale in this model was unity and the agreement in each case is reasonably good.

Another aspect of the salinity verification is the necessity to determine empirically the proper initial location of a barrier in the model. At the beginning of model operation the barrier is used to separate the salt and freshwater regions. The barrier is removed when the tide generator is started and a periodic steady-state salinity distribution is usually obtained within 10 to 20 tidal cycles.

4.3 SEDIMENT TRANSPORT VERIFICATION

Many estuary models have been designed to study shoaling and sediment transport effects. This involves the introduction into the model of special light-weight sediments which are capable of being moved by the tidal currents in the model. Because of the lack of geometric and dynamic similitude and the low Reynolds number of the model, there is no direct way of scaling rates and amounts of sediment deposition from model to prototype. This is an example of the necessity of developing *ad hoc* verification procedures. This consists of finding an empirical time scale for sediment transport. The time required for a change in sediment distribution in the model is observed and compared to the known time required for a similar change to have occurred in the prototype. This time scale may be considerably different from the Froudian time scale Equation (5.10). For example, in the Absecon Inlet model, the time scale for sediment transport was 1/675 while the Froudian time scale for the model was 1/50. The prototype period for verification was three years.



DISCHARGES AT CLYO GAGE:
JAN 12, 1936, 67,000 CFS
JAN 13, 1936, 72,000 CFS
JAN 14, 1936, 73,000 CFS
JAN 15, 1936, 71,000 CFS
JAN 16, 1936, 66,000 CFS

SAVANNAH HARBOR, GA.
CURRENT - SALINITY DATA
STATION 190
15 JANUARY 1936

Fig. 5.13 Vertical distribution of salinity and tidal current - Savannah Harbor. $Q_f = 71,000$ cfs. After Rhodes (1950).

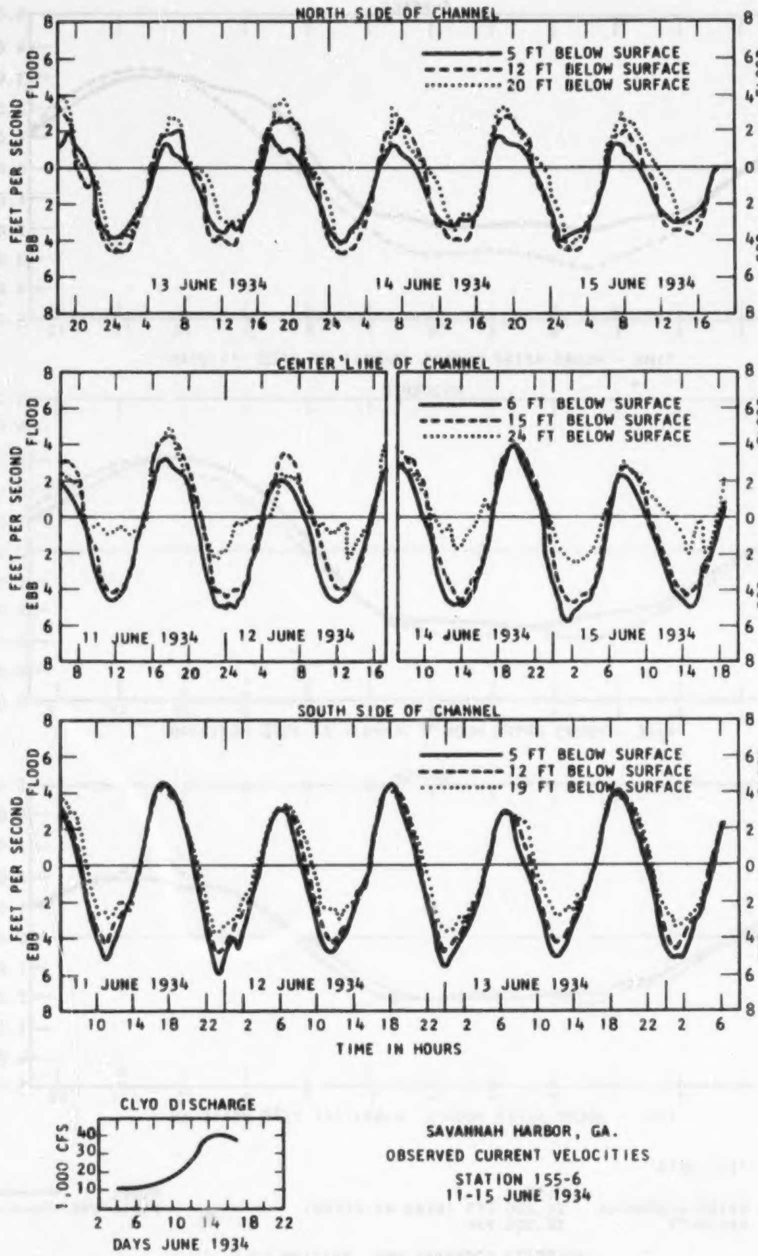


Fig. 5.14 Lateral and vertical distribution of tidal current - Savannah Harbor. After Rhodes (1950).

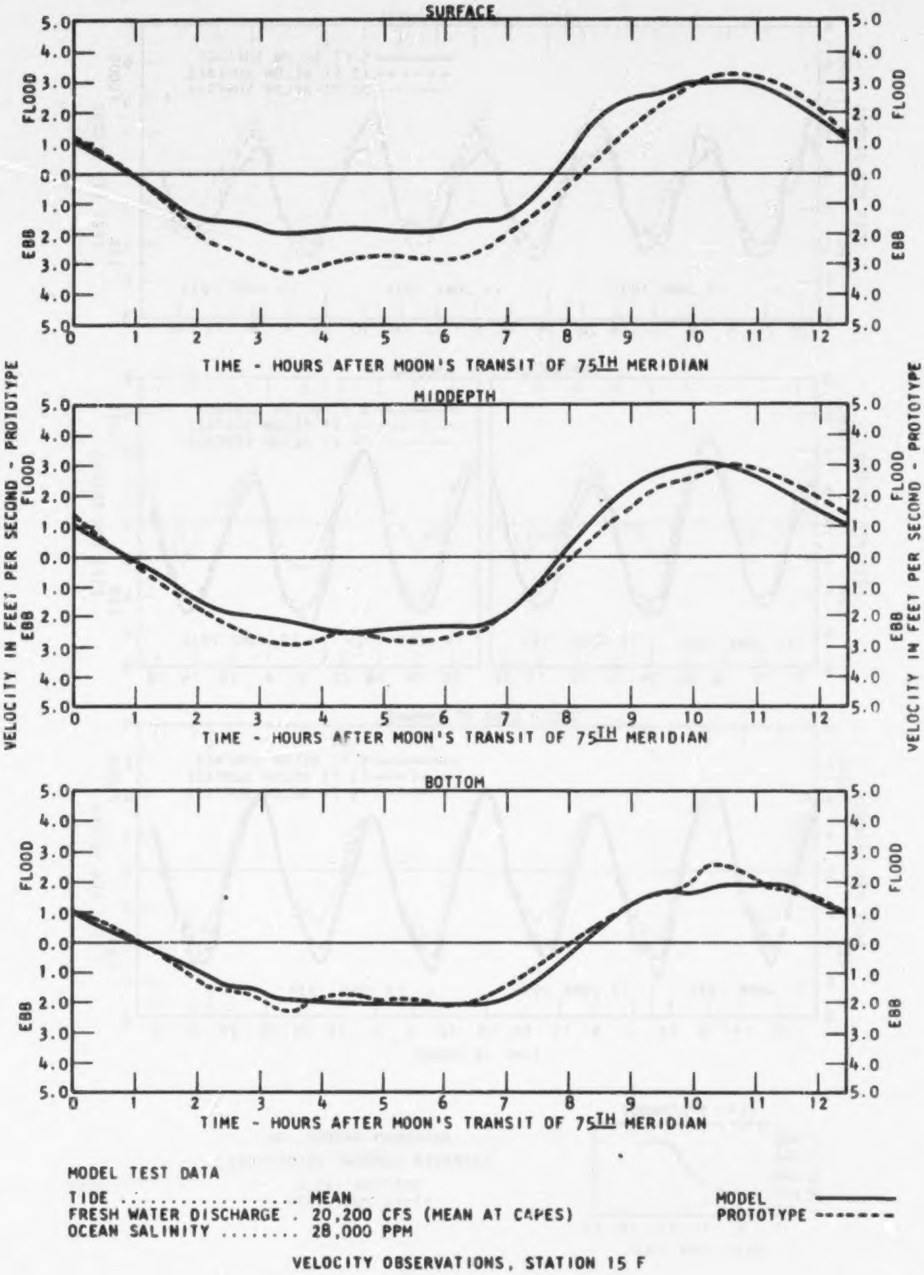


Fig. 5.15 Model-prototype tidal velocity verification - Delaware Estuary Model, Station 15-F.

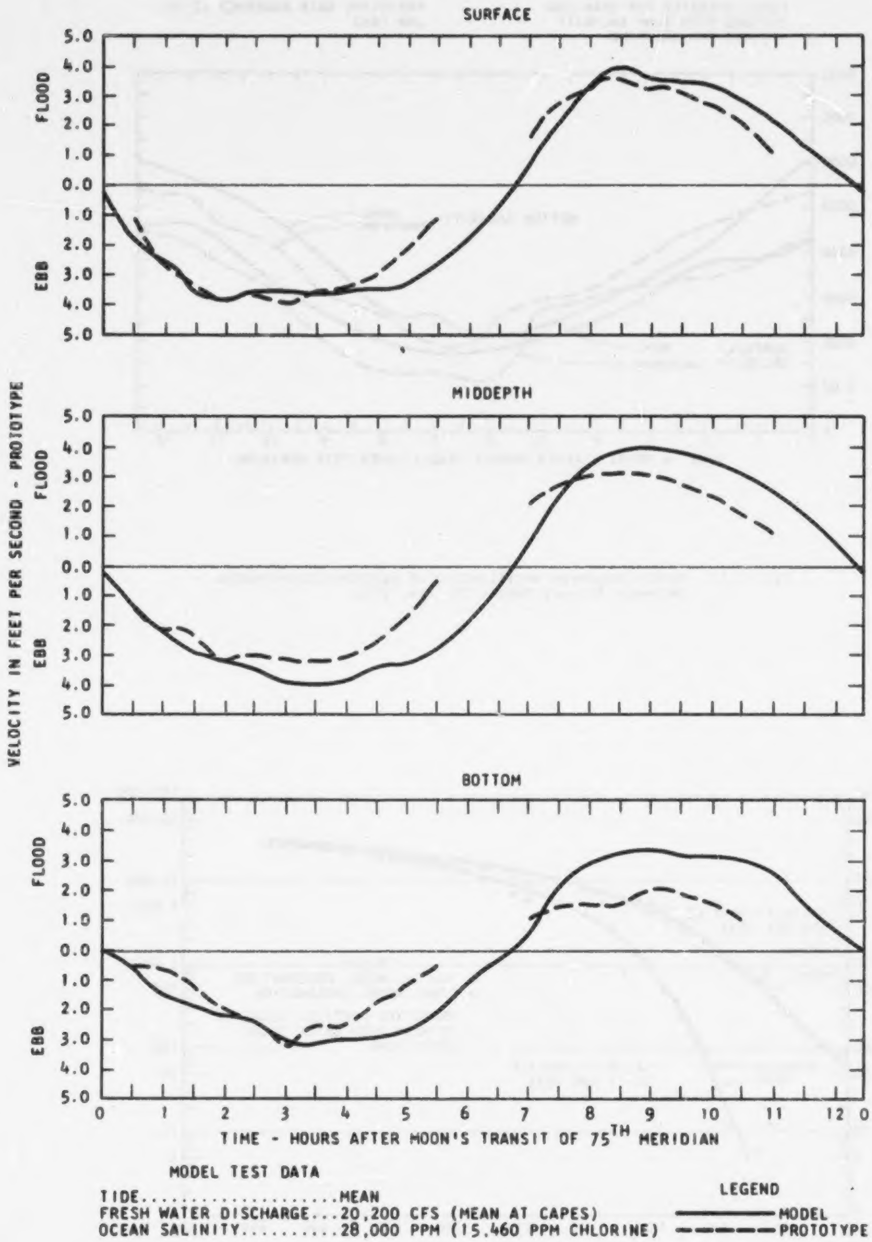
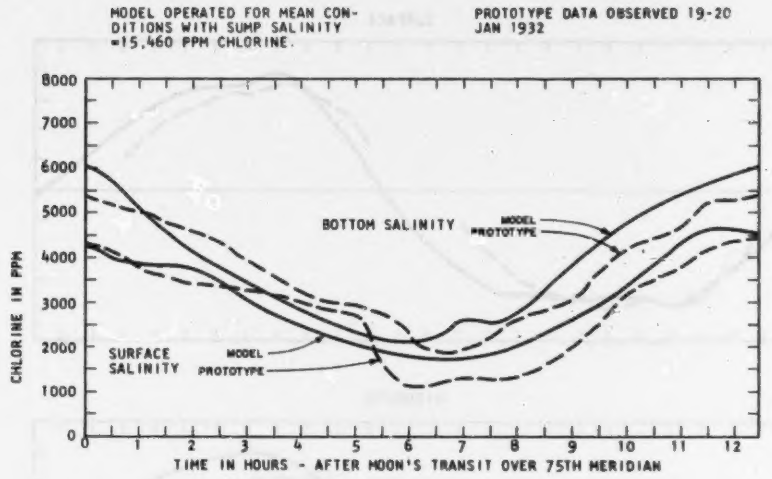


Fig. 5.16 Model-prototype tidal velocity verification - Delaware Estuary Model, Station 4-B.


MODEL OPERATED FOR MEAN CONDITIONS WITH SUMP SALINITY =15,460 PPM CHLORINE.

PROTOTYPE DATA OBSERVED 19-20 JAN 1932

Fig. 5.17 Model-prototype verification of salinity distribution - Delaware Estuary Model, Ch. Sta. 275.

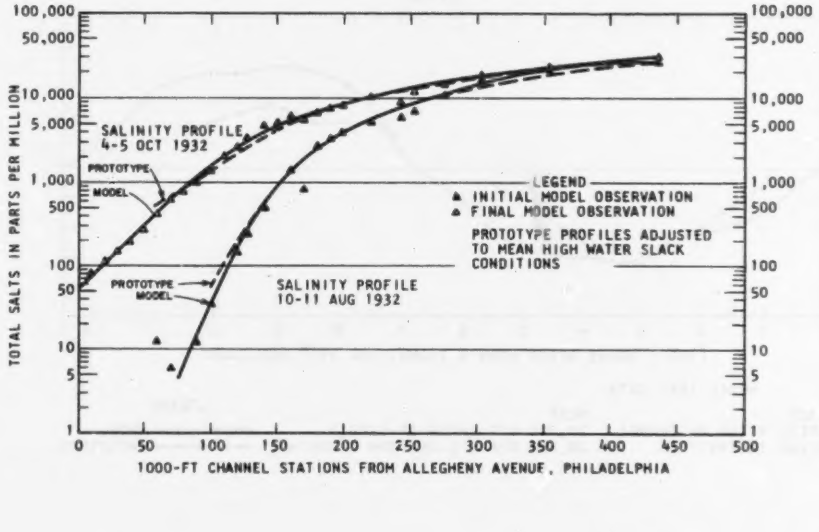


Fig. 5.18 Model-prototype verification of surface salinity profiles - Delaware Estuary Model.

5. DISCUSSION OF THE USE OF PHYSICAL HYDRAULIC MODELS IN ESTUARINE WATER QUALITY STUDIES

The use of physical hydraulic models for the investigation of estuarine water quality problems has an obvious attraction, compared to field studies, in terms of economy and speed of data collection. Physical models can be operated under controlled conditions and changes in effluent characteristics, location and discharge rates can be made very easily. The growing concern with water quality, coupled with the fact that physical models of many of our major estuaries are already in existence, has led to a rapid increase in model usage for water quality problems.

The undisputed success of physical models of complex estuaries in providing engineering solutions to important problems concerned with navigation has generated a high degree of confidence in these models. This confidence has been built up over a period of several decades by careful model verification procedures based on large amounts of field data directly related to the original purpose of the model. A review of the literature dealing with the application of physical models to water quality studies indicates that there is some danger of transposing confidence well beyond the demonstrated validity of such models.

Relatively few attempts have been made to explore the theoretical basis for the similitude of mass transfer processes in model and prototype. The important points are that estuary models are geometrically distorted (usually by a factor of 10 to 1) and that only gravitational-inertial similitude is guaranteed by the Froudian scale ratios for velocity and time. In most cases the only mass-transfer-related process subjected to model verification is the salinity distribution. The ability to reproduce salinity distributions in physical models is undoubtedly related to the fact that gravitational effects play a dominant part in the salinity-induced circulation. Mass transfer processes associated with initial dilution, turbulent diffusion, and dispersion depend primarily on internal fluid shears related to local velocity and turbulence distributions, none of which are assured by Froudian similarity.

The discussion in Section 3.2 of mass transfer similitude is based on an inspectional analysis of longitudinal dispersion. It is concluded that there is a large distortion of the one-dimensional dispersion process in the uniform-density regions of estuary models. Furthermore, the Froudian scales relating model-prototype times are such as to preclude the rate process scaling of non-conservative substances. These considerations suggest that water quality studies in physical models be approached with considerable care in recognition of potential sources of difficulty.

The earliest investigations of water quality problems in estuary models were concerned with the empirical determination of one-dimensional flushing and dispersion characteristics. The Delaware estuary model was used extensively for this purpose beginning in 1952 (Pritchard 1954, Interstate Comm. 1961, O'Connor 1962). One of the objectives of this type of study was the determination of dispersion coefficients for use in the one-dimensional, non-tidal advective mathematical models (see Sections 3.4 and 3.5 of Chapter II). In the Delaware model, dye was injected in the upper freshwater tidal portion in the vicinity of Philadelphia. In the light of present-day knowledge, both the validity and the need for such tests is highly questionable. The validity is questionable because inspectional analysis indicates distortion of the dispersion effect. Furthermore, the model had not been verified for mass transfer processes above the region of salinity intrusion; and in addition, the model dye concentrations must be corrected for dye loss in the model. The need is questionable because the real time mathematical model (Sec. 3.2 of Chapter II) relates the dispersion characteristics to the tidal velocities. Therefore, one-dimensional concentration distributions can be calculated without resort to field or hydraulic model dispersion tests.

A second group of water quality investigations in physical hydraulic models is concerned with variations in concentration distributions brought about by changes in the location and geometry of an effluent outfall structure. Potentially this is one of the most important areas of application of the physical model. The concentration distributions are three-dimensional and their prediction by means of a mathematical model is generally not feasible unless the geometry and current patterns can be greatly idealized. Beginning about 1956, the Delaware estuary model was used for the study of the dispersion of effluents from two industrial plants (WES 1957a and 1957b). In each case it was desired to investigate the benefits to be obtained from changing from a shoreline outfall to a submerged outfall extending laterally to a deeper portion of the estuary cross section. The site of one plant, near Philadelphia, was above the region of salinity intrusion, while the other was just below the limit of intrusion for normal freshwater inflows.

Recently an outfall location study was undertaken on the model of the James River estuary (Bobb and Brogdon 1967). Tests were made of three submerged sewage outfalls located 4000, 8000 and 12,000 ft. from the shore, the latter being in the middle of the estuary section above Newport News. The model extends from the Atlantic Ocean at Cape Henry to the head of tide at Richmond, Virginia. The usual scales of $L_r = 1/1000$ and $Y_r = 1/100$ were used and the entire model is 550 ft. long and 130 ft. wide at the widest point. The difficulties associated with determining the effect of a total lateral change in outfall location of 8 ft. in the model are readily appreciated. No local verifications were made for either the James or Delaware outfall model studies. It is therefore difficult to assess the quantitative significance of the local concentration distributions observed in the model. The state-of-the-art is such that we are not able to evaluate the effect of a 10 to 1 distortion of the side slopes of the estuary on the initial dilution and entrainment of an outfall structure.

The Savannah estuary model (Simmons and Rhodes 1965) has been used to determine the effectiveness of several proposed closure dams in reducing the amount of pollution entering the Wilmington River from the City of Savannah sewer outfall located in Savannah harbor. A continuous release of dye simulated the sewage effluent and sampling was performed periodically for 50 tidal cycles in the model to determine the resulting concentrations throughout the study area. There were no verification tests related to the effluent discharge and the model results were not adjusted for dye decay, loss in the ocean basin, or adsorption on boundaries of the model. Such model results are very useful in a comparative sense.

An extensive series of water quality related model tests have been performed in the San Francisco Bay model in recent years. The original series of dye dispersion tests began in 1960 for the purpose of determining the pollution effects of proposed salinity control barriers within the bay area (O'Connell and Walter 1963). In these tests dye was released at various locations during one tidal period in the model. Computational procedures were suggested for correcting the measured dye concentrations for dye loss in the model and for estimating the "conservative" concentrations to be expected for a continuous release in the model. A uniform prototype decay rate constant was then applied to the corrected model data for the purpose of simulating prototype BOD distributions. No verification results were reported for these tests. Later model tests (Bailey *et al*. 1966, Bailey 1966) were conducted to study the pollution in the northern arm of the Bay resulting from the discharge of the proposed San Joaquin Valley Master Drain. Again, model data were corrected by estimating dye losses due to decay, adsorption and absorption. Field studies were made for model verification purposes by means of dye injection and extensive sampling in the prototype. The primary difficulty is in the determination of the appropriate dye loss correction factor for the field data. In the absence of an accurate means of evaluation of this factor, a normalizing procedure was used in which ratios of prototype-to-model concentrations were determined for several locations at various times. The final comparison of model-prototype data indicates a sizeable variability as shown in Figure 5.19. In general, the prototype concentrations are lower than those predicted by the model;

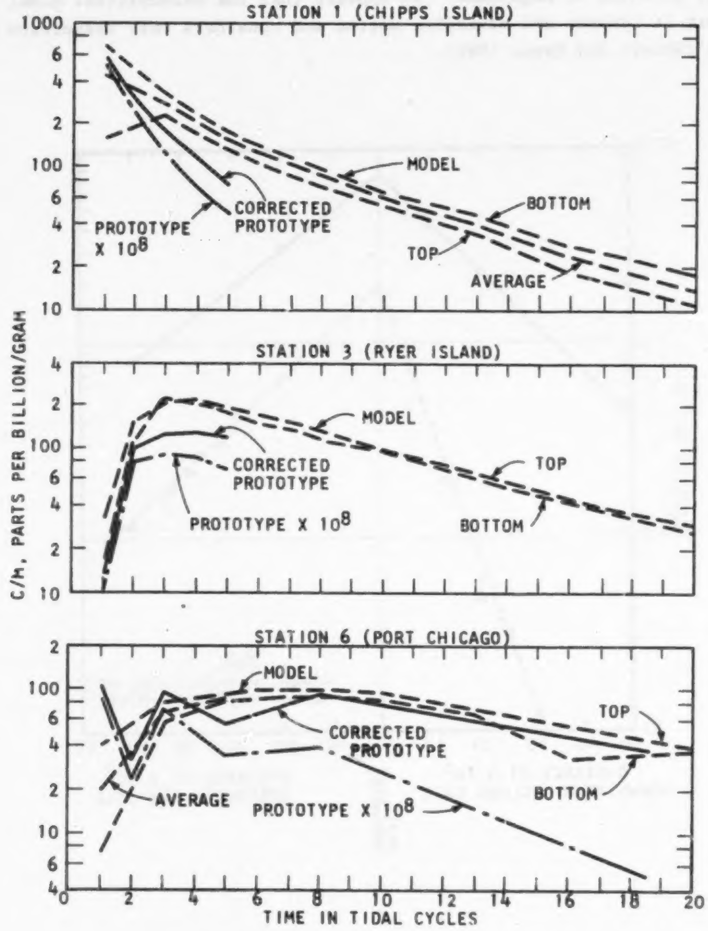


Fig. 5.19 Verification of the San Francisco Bay Model by comparison with prototype dye dispersion patterns. From T. E. Bailey, C. A. McCullough, and G. G. Gunnerson, Mixing and Dispersion Studies in San Francisco Bay, Proc. ASCE, 92, No. SA 5 (October 1966), pp. 23-45. Used with permission of American Society of Civil Engineers.

however, the order of magnitudes are reasonable. This represents one of the few attempts at direct model verification of water quality parameters and it provides an excellent illustration of the difficulties involved. The fact that the dye injection locations were within the region of salinity intrusion undoubtedly was an important factor in the ability to achieve some degree of verification.

Recently, the San Francisco Bay model has been used for effluent disposal tests in the southern arm of the Bay (Lager and Tchobanoglous 1968). No verification studies were conducted. However, an attempt was made to compare the results of the hydraulic model with the predictions from a mathematical model. The results, as shown in Figure 5.20, are inconclusive as they differ by an order of magnitude. It appears that the mathematical model is oversimplified in that it ignores all advective motion and considers only dispersion and a first-order decay term (Stover and Espey 1969).

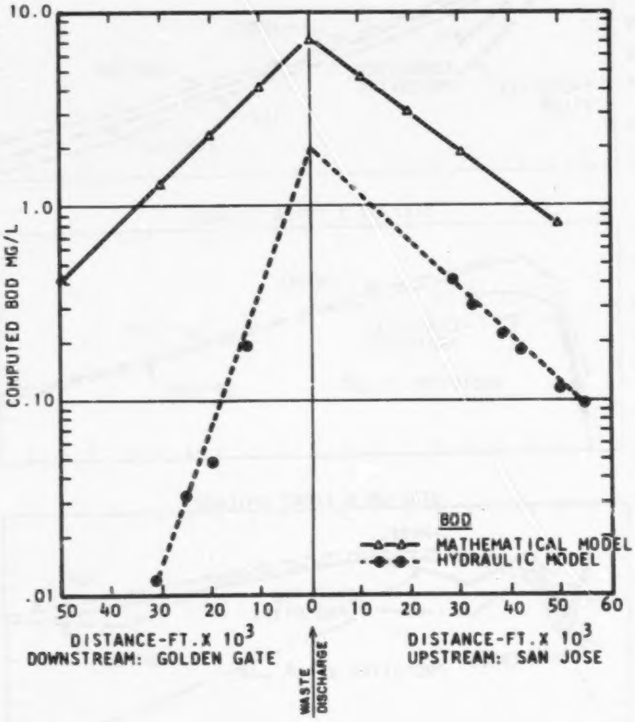


Fig. 5.20 Comparison of computed BOD distributions for measurements in San Francisco Bay Model with results from a mathematical model. From J. A. Lager and G. Tchobanoglous, Effluent Disposal in South San Francisco Bay, Proc. ASCE, 94, No. SA 2 (April 1968), pp. 213-236. Used with permission of American Society of Civil Engineers.

6. SUMMARY AND CONCLUSIONS

The similitude conditions for tidal motion in distorted hydraulic models are well established through the Froude scaling laws. Experience with the large number of tidal models constructed has shown a good reproducability of the essential features of tidal motion. Although Reynolds numbers are of the order of 10^3 less in the model than in the prototype, the boundary resistance is primarily in the rough-turbulent regime and similarity is achieved through roughness adjustments in the model.

The analytical basis for similarity of salinity intrusion in both stratified and well-mixed estuaries is discussed. For the stratified case (the classical saline wedge), the requirements are (i) equal density difference in model and prototype, and (ii) a condition relating the ratio of interfacial shear stresses to the horizontal and vertical scale ratios of the model. By making an assumption as to the nature of the interfacial stress in model and prototype, it is shown that the similarity condition is satisfied for only one value of Y_r, if L_r is fixed. For the well-mixed case, it is shown that the ratio of pseudo-dispersion coefficients describing the one-dimensional gravity-induced circulation is given by $E_r' = Y_r^{1/2} L_r$ within the region of salinity intrusion. There is no strict necessity for density difference equality in model and prototype although the practice has been to make the density differences equal. Similarity of the salinity intrusion can be guaranteed only by verification of the model with field data. The verification process is assisted by employing vertical strip resistance elements which promote vertical mixing in the model.

The analytical basis for the similarity of dispersion processes in tidal regions consisting of fresh or homogeneous saline water (no longitudinal density gradients) is examined. It is shown that the ratio of dispersion coefficients, given by $E_r = Y_r^2 / L_r^{1/2}$, is incompatible with the dispersion coefficient ratio E_r' in the well-mixed salinity intrusion region. It is concluded that the dispersion process in hydraulic models of uniform-density tidal regions is distorted by virtue of the physical distortion of the cross-sectional geometry. Because of the Froude time scale requirement, it is not possible to simulate directly the distribution of non-conservative substances in physical models.

The necessity of model verification, using field data closely related to the phenomena to be studied, is discussed. Examples of model-prototype verifications and the associated difficulties are presented.

Examples of the use of physical hydraulic models of estuarine systems for problems related to water quality control are presented. In view of the very limited experience in direct verification of model-prototype water quality studies, generalized guidelines are difficult to formulate. Physical model investigations are of value in certain comparative studies of three-dimensional concentration distributions. The use of physical models in the determination of one-dimensional concentration distributions appears to be of limited value in comparison with available computational techniques. Additional attention should be given to the need for model verification of water quality parameters, although it is recognized that quantitative verification is difficult due to the necessity of independent dye loss corrections in both model and prototype.

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DISCUSSION

HARLEMAN: Hydraulic models, that is, physical hydraulic models, have been around for a long time, roughly since the 1880's. However, their use in terms of water quality problems is much more recent, almost, perhaps, within the last ten years. I began their discussion by considering similitude of momentum transfer processes in tidal motion, because it seems quite clear to me that if we are going to deal with water quality processes in estuaries in terms of a physical hydraulic model, that first of all that physical hydraulic model must do a good job of simulating the basic tidal motion. As has already been emphasized many times today, the importance of the advective motion cannot be overlooked. And this basically boils down to a concern with Froude scaling. Also we should observe that we are always talking about distorted models, because I think it goes without saying that the possibility of building a geometrically undistorted model of an estuary is rather remote. They are all distorted, usually by a factor of ten to one, almost a universal factor, so we are not talking about small distortions but large ones.

The consideration of Reynolds number effects in relation to the tidal motion turns out to be not very important for the simple reason that the energy dissipation of both the model and the prototype is primarily in the rough turbulent regime, and is therefore very little influenced by the fact that the Reynolds number of the physical model is very much smaller than that of the prototype. In fact, for the typical scale ratio of 1/100, 1/1000, the model Reynolds number will be a thousand times less than the prototype. However, this is not of great importance simply because the frictional effects which are important in the tidal motion are not strong functions of the Reynolds number. They are primarily functions of the geometric roughness, and one goes to distortions of the geometric roughness in the model in order to achieve this type of similarity.

Then I went through the same type of operation discussing the similitude of mass transfer processes in models. This is one which has received surprisingly little fundamental attention, considering the number of times we have undertaken to study mass transfer processes in physical hydraulic models. We begin by considering the problem of similitude of salinity intrusion, and, to keep the problem simple, consider only two extreme cases. First, the saline wedge--and this is the simple saline wedge in which the upper layer remains fresh and the lower layer remains salt, without considering mixing or advection between the two layers. If you follow the process through again in terms of inspectional analysis, or conditions necessary for similitude, you find again that there are two Froude number conditions, the densimetric Froude number and the normal free-surface Froude number, which must be satisified simultaneously. This can be done if you keep the density ratios the same in model and prototype, as indicated in Equation (5.27). Secondly, making some assumptions about the nature of the interfacial shears, which in these cases are probably strongly dependent upon Reynolds number rather than geometric roughness (since we are talking about a fluid interface rather than a physical rough boundary), I have simply made some speculation on the fact that if you choose the distortion ratio properly as indicated by Equation (5.31) that you could achieve similitude. It is interesting to see that if you take a length ratio of 1/1000, based upon these assumptions the appropriate vertical scale is 1/150, which is fortuitously close to the thing that has been evolved over many years of deciding that generally this order of 1/1000 horizontally and roughly 1/100 vertically seems to work. This indicates a physical reason why this works in the saline-wedge estuary.

Then we go to the other other extreme, the fully mixed estuary. We go through the the process of taking the simple salinity equation for the variable-area estuary, Equation (5.32), putting it in a dimensionless form and looking at the magnitude of the coefficient which appears as this one-dimensional dispersion coefficient for salt divided by velocity and a length, and conclude that numerically they must be identical in model and prototype if we are to have similitude of the mixed estuary kind of salinity intrusion.

This is not of any great analytical consequence because, as most of you probably know, the achievement of similitude of the salinity intrusion regions (assuming now that we are talking about a mixed estuary) has generally been one of brute force. You cut and try, and adjust and snip and bend wire strips, and put in a great deal of blood, sweat, and patience, extending over a period of a year or two, of simple adjustment-verification until you make the model duplicate or replicate as well as you can, and you decide that now it's good enough and stop. So it is essentially a forced verification. You always have field measurements and you always adjust until you make the model replicate those as best you can.

I conclude from this that here is a mass transport process which people that operate models generally have succeeded fairly well in replicating in these small-scale distorted models. However, I will observe that it is a process which is strongly dependent upon the density effects. The whole intrusion of salt water, even in the mixed estuary, is critically dependent on the density effects, and therefore it's probably that the ability to duplicate this is related to the fact that we are achieving similitude with respect to gravitational effects, basically in the tidal motion. Since the salinity intrusion is also a gravitational-type circulation process, it is possible to duplicate this. But I think that the greatest fallacy that we have fallen into in the use of physical hydraulic models, is to assume, because we have replicated the salinity intrusion, that all other mass transfer processes are therefore going to be correct. That assumption is by no means valid.

We only have to proceed now to consider the similitude for mass transfer processes in regions of uniform density. By that I mean I don't care whether it is all salt water or all fresh water, but we're not going to have any density gradients. In going through that and looking at the scaling relationships for the one-dimensional dispersion, a la the Taylor-type equations, we see there is a vast difference in the scaling for this type of dispersion as opposed to the salinity-intrusion type of mass transfer. It turns out that the effect of the distorted hydraulic model in the non-salinity-intrusion regions is to introduce a very high distortion of longitudinal dispersion effects. The reason behind this, I think, is shown in Figure 5.9. This is a simple picture of the cross section of an estuary represented by Section A, and the cross section of that estuary as represented by Section B which is what you have in a ten-to-one distortion. It is quite obvious that the dispersive effects we are talking about now are primarily related to the details of the velocity distribution in the cross section.

Be that as it may, the question then comes to the use of physical hydraulic models in estuarine water quality studies. Now there is obviously a great attraction to the use of the physical hydraulic model, especially since so many of them already exist.

They have been built to study shoaling and sedimentation problems, and they are there, and so there is obviously the important question: why not use them for water quality studies? I have tried to present hopefully a fairly objective viewpoint of this. But the general opinion that I have is that you must be extremely careful in doing this whenever the process that you are looking at has involved a mixing or dispersion-diffusive process, because we now come back to the Reynolds number difference and the fact that we are talking about Reynolds numbers in the models which are three orders of magnitude less than those in the prototype. It isn't just a question of saying that since we had salinity intrusion agreement, everything else is going to be fine. I have given some examples of some of the things that have been done, and simply raised some questions.

I do not believe that we should at the present time use physical hydraulic models for the purposes of determining one-dimensional longitudinal dispersion coefficients, for the simple reason that the distortion effect is there. Furthermore, I think we can adequately estimate these, and we have already shown that if we use them in real time models they are not so important. So I think we should not use physical hydraulic models for the purposes of measuring one-dimensional dispersion any more than I think we should make field tests to do the same thing.

Potentially the most important area of application of the physical model is in determining concentration distributions which are three-dimensional. And this is obviously the point that is most difficult to do analytically, and so it would be nice if you could do this in a physical hydraulic model, especially if it already exists. As an example I quoted the outfall location study undertaken on the model of the James. The entire model is 550 feet long and 130 feet wide at the widest point. The outfall studies that they were doing involved moving the outfall a total of eight feet in that model. I think you have to raise very serious questions whether you have replicated the velocity structure in this ten-to-one distorted model (which means that you have distorted the slope of sides of the estuary by a factor of ten) sufficiently to study the effect of moving an outfall a total of eight feet out into the section. No verifications were done of this type of thing. It was simply a faith operation and everyone must draw their own conclusions.

I have also cited the rather extensive series of water quality model tests which have been undertaken in the San Francisco Bay model. Now here you come to the usual technique of making dye injections into the model. These have been made as instantaneous (so-called) injections, some of these so-called instantaneous injections extending in time over one model tidal period, and then others being so-called continuous injections.

It is pointed out in here that in dealing with a non-conservative substance in the model, due to the time scale involved, there is no possibility of duplicating the time scale of decay events, unless you happen to have a substance which had a decay rate exactly, say, one hundred times that of the prototype. If you have 1/1000 horizontal and 1/100 vertical it requires a decay rate of 1/100, a hundred times greater for the model substance. Well, dyes in the model don't decay a hundred times faster than Rhodamine in the prototype obviously, so that you have to unravel from these model tests the decay in the model, which is, in many cases perhaps, largely absorption of the dye on the boundaries of the model. This is extremely difficult if you are losing mass to the so-called ocean basin. In that case I really know of no way that you can truly unravel and determine the model decay rate precisely, because what you would presumably have to do is determine the model decay rate, correct your model dye data to a conservative substance, scale that up to the prototype, and apply prototype decay rates. This becomes an extremely difficult and messy operation, and I don't think it should be undertaken lightly without major consideration of what you're getting into. The attempts at verification with field data, I think, are somewhat inconclusive, basically because of these difficulties of really unraveling what is really decay and what is simply loss of substance at the ocean boundary, in many of these cases.

In summary, I suppose it appears somewhat pessimistic, but I think it is important to emphasize the factors which have to be considered, and I think that what has been largely lacking in the literature is just this type of being a little pessimistic. I do not make the statement what we should clearly give up all of these, but I think that we have too often simply proceeded too much on faith, without a real attempt to sit down and say what are the problems and whether it is worth trying to overcome them. I'm certain in many cases it may be, but it is by no means a cut-and-dried question.

PRITCHARD: I certainly would agree with Don. He was the first one to point this out. There has been considerable argument for many years, but I think that it is generally valid that in this matter of the freshwater region, the uniform-density part of the model, I think that we certainly agree that we shouldn't use the model to compute one-dimensional flux or dispersion characteristics. (Remember when we say uniform density, we're talking about horizontal as well as vertical, and not just vertical. That is, the advective effects will still be there even though they are pretty thoroughly mixed vertically.) Much of the work that I've seen done on these models is again dealing with practical problems where one is concerned primarily with what happens within roughly a tidal excursion of the discharge, and admittedly one is left with considerable uncertainty as to how well the system matches.

In my experience with verifying these models, or what's called verification which is really adjustment, the practice is to insert roughness elements, and these roughness elements are inserted primarily on the basis of having the tidal dissipation correct. There are empirical relationships with which one could build a model now and put in almost the right number of roughness elements. Now, if you have a number of tidal observations so that you know the phase and amplitude of the tide at a large number of places in the bay, you use these in verifying the model or adjusting the model so that you get the right tidal height, the right tidal phases through the system. Then the next step is to look at observations of velocities in the field and in the model. Now here we get into a problem of considerable greater magnitude, from the standpoint of the difficulty of measuring a velocity versus time in the field and in the model, and the fact that there's going to be considerable more variation in the current structure due to differences in winds, etc., in the prototype from time to time, so that the comparison between these is more difficult. But the general tendency is to now redistribute the roughness elements locally without changing the total amount of roughness, that is, the total energy loss, to reproduce the currents, or to better fit the current velocities that are observed. This is all done with fresh water in the model, not trying to simulate the vertical shears due to density difference at that stage, but primarily the lateral and longitudinal distribution of the vertically averaged current.

Once the model adjuster says, "This is as far as I can go. I'm tired," then he puts seawater in the ocean sump, and lets river water come in at the proper rate, and looks at what the salinity distribution is. My experience has been that at that stage there is very little further adjustment to the model. The model does behave correctly salinity-wise, except, as you have pointed out, there are some times when they have pointed out that the comparison is pretty good, and there are some details that look suspicious.

HARLEMAN: In general it's pretty good, I would agree.

PRITCHARD: But, in general, the salinity distribution is pretty good without special adjustment for salinity. The adjustment is for tidal height and tidal velocity.

HARLEMAN: But there is still an empirical factor there. They could have gotten that adjustment with stones on the bottom, but by using strips which give the same energy dissipation they have evolved also getting the salinity. It is not automatic because you could do the tidal replication against the stones on the bottom and you would not have any vertical exchange, which the strips introduce. So it's empirical.

PRITCHARD: Right. In any case, once they've done that with the strips they end up with, apparently as far as the scale of phenomena that controls the salinity, the right kind of vertical mixing. You see, you not only have to have the gravitational effect, you have got to have the vertical mixing between the counter-flowing layers, counter-flowing now with respect to a tidally moving reference system. My point would be that for those problems of dispersion, or of concern with the distribution of properties, if you're in a section of the estuary in which these processes of horizontal advection and vertical mixing are the important processes as far as an introduced pollutant is concerned, then I would expect that the three-dimensional distribution of the pollutant would be similar. Now the problem is that there has not been adequate verification, adequate comparison between model and prototype, that would lay this question to rest. I think that this is an unfortunate situation. So my argument would be here, not that I would disagree with Don's cautions, and I don't say this from the standpoint of promoting the construction of hydraulic models solely for water quality studies, but since there does exist models for other purposes, it behooves us to lay this question to rest, or at least to get enough field data, duplicate sets of observations in model and prototype, on the matter of the distribution of an introduced material somewhere within the estuary. I'm now talking about within the part of the estuary in which there is a variable salinity distribution with distance.

HARLEMAN: I agree with you. I think the problem is that whenever you do this, that is, you put dye in the model and dye in the field, you have these correction factors which somehow always seem to obscure the answer finally as to whether really it is verification or it's really an inability to determine these two different decay factors.

PRITCHARD: Yes. I have somewhat of an opinion about the decay, these so-called dye decay factors. One thing is that one can select dyes which are much less absorbent than some that have been used, both in the model and in the prototype. And second, I think that the reason for loss of dye in many cases, particularly in the field, is the fact that one loses dye outside, because it goes to levels of concentration below the background. It's very similar to the problem that has arisen with respect to people using field studies of thermal distributions to deduce that the cooling coefficients in nature are much higher than those that either theoretically or empirically come from cooling ponds. Essentially a good deal of the heat is mixed to such low concentrations that one says that it is zero concentration. And it is not. You don't draw a zero concentration line.

We've done field measurements for a month at a time, introducing dye into an estuary of considerable size and telemetering the distribution, and we have found 110% of the dye. Now this indicates the uncertainty in these kinds of processes. It also indicates probably some variation in the background. But in other cases we have not been able to find all of the dye, and I think we can readily show by simply a very slight adjustment to what we call the background (there always is a background here) that we can account for all of it.

I'm just not convinced. I think that I would rather make the comparisons directly, at least if I pick dyes that I have pretty good faith in as far as a rate of decay. I agree that that has been a problem. I think it need not be a problem.

HARLEMAN: I think one can make a good case for getting reasonable results especially within the salinity intrusion region if things are fairly one-dimensional, but I think I would point out that it is precisely those problems which we can calculate, and we don't need models or field tests to do. It is the three-dimensional local problems that we can't calculate that we would like to do with models, and I simply have to come back to the James River where the thing was 130 feet wide and they moved the outfall a total of 8 feet. To ask the real question, is this, in a ten-to-one distorted model, providing the three-dimensional answers that you think you are getting?

PRITCHARD: Do you mean whether you can really tell the difference between the discharges?

HARLEMAN: That's right.

PRITCHARD: That I would certainly question.

HARLEMAN: If it's one-dimensional, we don't need to do the model tests. We can calculate it.

PRITCHARD: The question is that the model may not be able to tell the difference between those two sites. But what about, let's say, the absolute prediction with respect to what the distribution was from one side, compared to how well you can produce that three-dimensional distribution any other way?

HARLEMAN: That seems to me the place where the model has the greatest potential, and where we don't have really any good information on how good it is.

PRITCHARD: Yes, that is what I am saying. Since inherently the model is three-dimensional to begin with, although distorted three-dimensional, we ought to not abandon it, until we are sure it has to be abandoned, for those problems in which its unique features would be valuable.

WASTLER: I would like to add something to this. On the Savannah, we were doing an enforcement study in 1963, and we did duplicate dye releases in the prototype, and the results were quite good. But it was not possible to make a mass balance on that because of the characteristics of the kind of system, which is half marsh. And then when we were working in Charleston, we had a half-scale model on the Charleston system which the Corps built and verified against their original data. We did not do dye tests in that. However, we had five field surveys in which we had taken time series data of some 30 samples at three- or four-hour intervals over the course of three-quarters of a year.

What we did was get the Corps to run the hydrograph in the model, and then we sampled the model precisely as we had sampled the prototype. We found that the results were extremely good at the high flows but they fell apart at around 10,000 cfs, which we never reported because what we were worried about was down below that and we had to reach our conclusions by other ways. But at least as far as the high flows, that half-scale model worked fine.

HARLEMEN: What do you mean by half-scale?

WASTLER: It was 1/1600, scaled down to half the physical size of the Savannah model. That was one reason that we tried to do this type of verification, because we weren't at all convinced that half-scale would work. As it turned out it didn't. Also, we found that the quality of the hydraulic model data went up considerably on the Savannah and the Delaware and a couple of others. Also we convinced the Corps of Engineers that seconds were important in their sampling procedure in the model.

HARLEMAN: With a time scale of ten minutes per tidal cycle, it can be very important.

WASTLER: I stop-watched them a few times, and they were anywhere within 10 seconds, 15 seconds, in their normal thing. We got it down to little flashing lights, to take it right then, and the data improved tremendously.

PRITCHARD: Interesting. Just one comment. Don had pointed out the fortuitous results that scales of 1/1000 and 1/100 seemed to be right for certain scaling features that he's described here, one where it came out 1/1000 and 1/150 as being the right scale for one of the requirements he had. It is interesting to note that for a one-to-one similarity in cooling coefficients across the surface, 1/1000 and 1/100 is the proper scale. If you have other scaling, if you're dealing with thermocouples, you have a correction to the cooling coefficients. It involves the depth scale and time scale, but it involves the depth scale in a certain combination that comes out to be 1/1000, 1/100. It's not just a ten-to-one distortion; the actual scaling comes out right. And if you work in a bigger model, a model like 1/300 and 1/30, your cooling coefficients are off by about a factor of two.

VLASTELICIA: Can you actually model thermal exchange problems in a hydraulic model?

HARLEMAN: Yes. It's mentioned briefly in here, one example, but certainly not given any great prominence.

PRITCHARD: Don and one of his students have done a model of a thermal release in Cape Cod Bay in which I think he has some reasonable confidence. There are models built of segments of the estuaries, which I have always been concerned about because they weren't complete estuarine models, but there is one done at Chalk Point. The data taken in the model was not very good, but, to the extent that can be compared, certainly was grossly different from what we have observed since the plant has been built, as far as the temperature distribution in the vicinity of the plant goes.

HARLEMAN: I think we come back to the point again that in most of the real problems it's the local dilution rather than the cooling that's the important factor.

PRITCHARD: Yes, and besides that, in the real problems, it's related to the momentum entrainment in the discharge, and this is a Froude-scale phenomenon which can be properly scaled in the model. The cooling term probably is incidental. It is interesting that it's the same, but it is not the important term. It's the momentum entrainment in the jet discharge, and that needs to be densimetrically Froude scaled so that this can be done in the model and prototype.

RATTRAY: There are a number of things here. I certainly agree with the basic thesis, that there is some concern about modeling the dispersion of any kind of thing in these hydraulic models. If I go back to an old paper I did, I did come up once with a relation for the roughening required for models with certain ratios of roughness lengths to depths and distortions. So there's a relation that can be determined. Actually, it turns out that in the model we have for Puget Sound, the roughness elements are effectively large compared to the depth of the system, the distortion is 1/40, which is larger, and we get very reasonable tidal representation with no additional artificial roughening.

HARLEMAN: Osborne Reynolds had, I think, distortions of 1/300 and he got pretty good tidal representations, too. Tidal representation I think you can get.

RATTRAY: It can be understood why and when you need to put artificial roughness in, and how much. What I guess I'm saying is if you could really model it, you wouldn't have to do the empirical tests.

The other thing is, in the things we've been talking about, really what the roughness elements are doing is generating turbulence, and through the distorted model and distorted roughness elements, you're generating turbulence that's different in the model from that in the prototype. Basically, its linear dimension will be distorted in the vertical over what it would be in the prototype. Now as far as the mean salinity distribution, if it is the largest scale of turbulence generated that is responsible for that (in addition to there being in flow which is Froude-scaled and tidal flow which is Froude-scaled) then with a density ratio of one, you can reproduce the salinity distribution automatically. This is essentially what has been found out. For other scales, however, smaller scales, you have to worry about what happens to turbulence in these smaller scales, and there is a tendency towards isotropy as you go down the scale of turbulence, so you would no longer expect to have the same distortion in smaller scales as you would have in the larger scales. Again this was a concern that was brought out that I think is understandable. Basically, I think that the points brought out here are very important. There are limitations and some uses.

THOMANN: I have sort of a general overall comment. Once a few years ago Dr. Harleman so aptly pointed out the problems of utilizing the physical model, in the freshwater portions especially, for determining dispersion coefficients. I am much more pessimistic since that time about the use of such models for water quality work. I think the tendency in much of our conversation over the last hour or so on physical models has been to equate water quality with only such variables as salinity, dye or some kind of tracer. If you look at decay and interactive or coupled water quality variables, I can't for the life of me see how you'd ever be able to utilize a physical model for that, even for very simple water quality variables. I think if we list the dozen or so variables in which we would be interested in water quality, there are only relatively few that we could really even hope to make any inroads with the physical models. I'm much more than pessimistic in the use of physical models for water quality. I don't see how we can use them, for example, in any coupled system of equations. And as soon as we introduce feedback, it's even worse. The whole issue of reaction rates, scaling down bacteria. You just can't do those kinds of things.

VLASTELICIA: Something that would be important, I think, to us would be some coverage in this section about very small scale models and highly distroted models that maybe we could afford to build. We couldn't afford to build the kind the Corps does. But Dr. Rattray's model has shown some net circulation patterns. It would be valuable to have a management tool like that. And you could maybe afford to build one, if it is highly distorted and small scale.

HARLEMAN: Well, I simply worry about its use in local effects. If you want to use it to study the kind of problems that involve the gross effects, I have the opinion that maybe you can do it by calculation.

RATTRAY: I even go further than that. I think Puget Sound may be the only body of water in the continental U. S. where it could be possible to even make one of that scale.

VLASTELICIA: I think some of the Alaskan estuaries might also eventually, I would suspect, be worthwhile modeling that way, to make some management decisions. I know an instance where a model showed that dyes put in at a pulp mill outfall location actually moved up at mid-depth into a valuable spawning area for bottom fisheries. And there's something I don't think you could measure ahead of time.

RATTRAY: We knew that was going to happen, but we couldn't convince others until we did it in the model, even though the model didn't represent it accurately.

CHAPTER VI

SOLUTION TECHNIQUES

1. ANALOG AND HYBRID TECHNIQUES

James A. Harder

1.1 INTRODUCTION

Digital computers are now sufficiently familiar so that there is no need to give an introduction to their characteristics. Their very real advantages in many areas of computation, their essential role in some areas, and the vigorous selling programs maintained by computer manufacturers have tended to obscure the somewhat older computational techniques of analog computing, analog simulation, and even hydraulic modeling. Analog simulation and analog computing have had to retreat, in a figurative sense, to those particular areas where they offer an advantage in convenience or cost over digital computing. The kinds of problems where their specialized advantages show up in the strongest way have the following general characteristics:

(1) There are only one or two dependent variables.

(2) The accuracy with which prototype measurements can be made does not warrant a high degree of accuracy in the computations.

(3) A principal problem is that of constructing a workable model, which has coefficients or parameters that can be adjusted so that a satisfactory degree of agreement in behavior is obtained between the model and its prototype.

(4) The number of adjustable coefficients or parameters is sufficiently large so that the integrative function or 'intuition' of the human mind can be brought to bear with advantage.

While there is no theoretical limitation on the number of independent variables that can be linked together in analog computations, certainly the advantage of digital computers is strongest when many variables must be handled at the same time. No one today would realistically suggest that analog computers be used to solve sets of linear equations.

Accuracy is a characteristic of digital computers, whereas analog equipment must work with errors of between .01 and 1 percent. A high cost premium obtains when errors must be kept at the lower of these figures. However, the accuracy with which tidal flows and pollutant concentrations can be measured in prototype estuaries is an order of magnitude less favorable than these figures, and it does not seem reasonable to insist that overall computational accuracy exceed that of prototype measurements by more than a factor of two or three.

The true accuracy of a water quality model, or other model simulating estuarine processes, lies not so much in the accuracy of the individual computations that go into its operation as in the accuracy with which it can duplicate the existing behavior of its prototype and the estimated reliability with which it can extrapolate that behavior to inputs and other conditions not yet experienced. "Goodness of fit," in the last analysis, must be subjective, though, of course, a degree of subjective judgement can be built into an objective evaluation by the use of weighting factors on errors. Differences in behavior between model and prototype will be distributed in both distance and time, and, of course, our toleration of error will be distributed too, but perhaps in a different way.

After a model has been built and tested, these errors can be graphed at leisure; certainly they will be instructive. However, it is during the testing and verification process that something may be done, in terms of adjusting the model parameters, to reduce these same errors. Anything that contributes to the facility with which the model can be adjusted to best duplicate its prototype's behavior is surely of the highest importance. It is in this phase of verification and adjustment that analog simulation and computation can make their most important contribution.

1.2 ANALOG MODELING

1.2.1 Analog Simulators and Analog Computers

The concise difference between analog simulators and analog computers is that simulators solve equations implicitly, in the sense that both the simulator (model) and the prototype are governed by the same equations (within simplifying assumptions), and thus the behavior of one is similar to that of the other. Analog computers, on the other hand, solve equations explicitly, in the sense that the equations must be developed and subsequently can be solved without regard to the setting up of a secondary model system. A more obvious difference is that the computer makes extensive use of operational amplifiers that perform addition, sign changing, and integration functions.

These differences will be made more explicit by two examples, each of which is of interest to those who would model estuarine processes of tidal flows and pollution dispersion. Experience shows that analog simulators are very useful in modeling tidal flows, whereas they have less success in modeling dispersion when convective terms must be included. In this latter case, the incorporation of some analog computing elements into a finite-difference scheme shows promise.

1.2.2 Analog Simulators for Tidal Flows

In constructing simulators, one looks for electric circuit elements that behave, relative to their own dependent variables, in a way similar to that of the prototype with respect to its dependent variables. The general criterion of similar behavior is that the two systems obey the same equations and that the equations are similar term-by-term. Very often this criterion is relaxed somewhat when it can be shown that some terms that have no counterpart in the parallel system can be neglected or compensated for.

We consider now the equations governing one-dimensional flow in tidal channels, noting that even in the process of setting up the equations, we have made assumptions that may have to be reexamined later. Particularly we here assume that water velocities can be averaged over a cross section, and that this average value can be used in the equations. We take flow as one of the dependent variables, for this is a quantity that is conserved; the other dependent variable is the water surface elevation. The independent variables are distance along the channel x and the time t. With these definitions, the equation governing the flow is as follows (a more complex derivation may be found in Harder and Masch 1961 and Paschkis and Ryder 1968):

$$\frac{1}{gA}\frac{\partial Q}{\partial t} + \frac{QB}{gA^2}\frac{\partial y}{\partial t} + \frac{Q}{gA^2}\frac{\partial Q}{\partial x} - \frac{Q^2}{gA^3}\frac{\partial A}{\partial x} + S_e = \frac{\partial z}{\partial x} \qquad (6.1)$$

The first four terms of this equation derive from the fact that the total derivative of velocity, required by the force-acceleration relationship, involves both the distance and time coordinates, and that the velocity is the ratio of discharge Q, and the cross-sectional area A. Since each of these latter variables are functions of distance and time, four terms result. The third and fourth terms constitute the "convective acceleration," and, in terms of energy, represent the convection of kinetic energy along the channel by virtue of the water velocity. The first of these four acceleration terms is by far the largest in tidal estuaries, and is ordinarily the only one simulated in analog models. Thus, some attention must be paid to the significance of omitting the next three. This significance will be developed in terms of a physical, rather than a mathematical sense. It is well known that shallow water waves, of which tide waves are examples, exhibit a wave velocity that depends on channel properties. This wave velocity, or celerity, is with respect to the water. Thus, the celerity is additive to the water velocity, and the tide wave generally travels faster relative to the banks than one would calculate from the formulas of elementary shallow water wave theory. The means of compensating for this effect will be discussed below, after a further discussion of the similarity relationships.

When we retain only the first term of Equation (6.1) there remains

$$\frac{1}{gA}\frac{\partial Q}{\partial t} + S_e = \frac{\partial z}{\partial x} \qquad (6.2)$$

where A is the cross-sectional area, g is the gravitational acceleration, Q is the discharge, S_e is the friction slope, and $\partial z/\partial x$ is the water surface slope. In terms of a finite length of channel Δx the equation is

$$\frac{\Delta x}{gA}\frac{\partial Q}{\partial t} + \Delta x\, S_e = \Delta z \qquad (6.3)$$

A second important equation expresses continuity of flow

$$\frac{\partial Q}{\partial x} + B\frac{\partial z}{\partial t} = 0 \qquad (6.4)$$

where B is the surface width and other variables are as defined above. In finite-difference form this equation is

$$\frac{\Delta Q}{\Delta x} + B\frac{\partial z}{\partial t} = 0 \qquad (6.5)$$

Note that time derivatives are not put in the form of finite differences, for in the analogs to be discussed, time remains continuous.

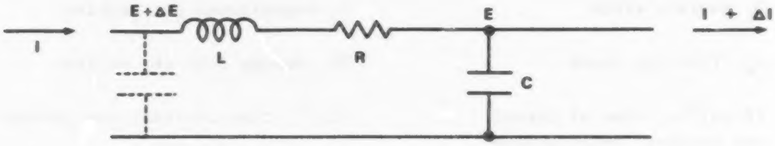

Fig. 6.1 LCR circuit for simulation of one-dimensional tidal flow.

Now consider the equations governing the lumped parameter electrical circuit shown in Figure 6.1. The equation governing voltage drops is

$$L\frac{\partial I}{\partial t} + RI = \Delta E \qquad (6.6)$$

where I is the current, L is the inductance, t is time in the electrical system, R is the circuit resistance, and ΔE is the voltage drop across the circuit. The equation governing the continuity of current is

$$\Delta I + C\frac{\partial E}{\partial t} = 0 \qquad (6.7)$$

where C is the electrical capacitance and other variables are as defined above. From these equations, scale factors relating the hydraulic and electrical parameters are easily derived and the following table of corresponding variables and parameters may be confirmed.

TABLE 6.1

Hydraulic Variable or Parameter	Electrical Variable or Parameter
1. Q, discharge	I, current
2. z, elevation	E, voltage
3. Δx, section length	(implied in capacitance and inductance per section)
4. A, cross-sectional area	1/L, reciprocal of inductance per section
5. B, surface width	C, capacitance per section
6. S_e, friction slope	RI, energy loss per section
7. $(B/gA)^{\frac{1}{2}}\Delta x$, time of travel per section, frictionless wave	$(LC)^{\frac{1}{2}}$, time constant per section

We return now to a discussion of the error introduced by neglecting the minor acceleration terms. It will be recalled that the actual wave speed relative to the banks is generally somewhat greater than the value that would be calculated from the channel properties because of the additive effect of the water velocity. Thus a frictionless tide wave advances through an estuary with the theoretical velocity $u + (gA/B)^{\frac{1}{2}}$, where u is almost totally determined by the wave itself, so we are not calculating independent effects. For example, the water velocity in a frictionless progressive wave is given by $u = y\,(gB/A)^{\frac{1}{2}}$, where y is the departure of the water surface from its mean value. Friction and reflections will alter the phase relationship of u and y, and friction will tend to reduce the wave speed.

When u is a small fraction of the wave speed, as is usually the case in estuaries, a reasonable compensation is to alter the value of the reciprocal inductance, and thus the implied cross-sectional area, to achieve the correct wave speed. This seems particularly appropriate when one considers that the cross-sectional area that must be used in the formula is not the gross cross section of the channel, but only the active part of the cross section where inertia is important; shoal areas that contribute storage, but where there is little longitudinal flow, must be excluded. This is equivalent to incorporating a factor that depends on the velocity distribution and which relates the actual momentum in the cross section to that which would be calculated on the basis of an average velocity. Estuary channels are often so irregular that little can be inferred directly about the value of the momentum correction factor. It can only be determined indirectly through an observation of the wave velocities.

Although friction has an effect on the wave velocity, its principal effect is that of attenuation. Unfortunately, at present we have no way of directly determining friction factors in estuary channels, for it is not possible to set up a steady flow condition from which we could determine Manning's n values from discharge and slope measurements. Instead we must infer friction coefficients from prototype measurements of wave attenuation. From these few remarks it should be apparent that one cannot take the simple-minded view that prototype measurements of cross-sectional areas or estimates of friction factors can be inserted directly into either equations or analog models with the expectation that good results will obtain. There is no shortcut around the verification process. A corollary is that the achievement of a correct wave velocity and attenuation in the model far overshadows in importance the inclusion of the minor acceleration terms; the latter can be compensated for, while without the first, no confidence can be placed in subsequent measurements in the model.

1.2.2.1 Simulating Hydraulic Friction The second principal term, the friction slope S_e , is nonlinear in two important ways. If we neglect bank friction, which is reasonable in the case of tidal estuaries, the equation relating S_e to the other variables is best given by the Manning equation

$$S_e = KQ|Q|/F(z) \qquad (6.8)$$

where $F(z)$ depends on about the 3.3 power of $(z - z_o)$ and where the absolute value sign is necessary for one of the Q factors so that the sign of S_e changes with that of Q . z_o is the elevation of a local datum approximating that of the bed. The factor K is introduced to account for bed roughness, assumed a constant. A nonlinear circuit element constructed of transistors has been devised that exhibits a voltage drop proportional to the current squared, with the correct sign convention, and having the requisite dependence on an external voltage proportional to $(z - z_o)$. This dependence on z is over a small range, so it is not difficult to achieve. This "square law" resistor has been described in Paschkis and Ryder (1968) and Harder and Masch (1961). The latest design is described in Paschkis and Ryder (1968).

An examination of Equation (6.8) will show the several effects of nonlinear friction. From the numerator we see that the frictional forces, proportional to S_e , depend strongly on the magnitude of Q ; a "square law" element correctly alters the friction in each channel element as the flows change during modifications of the model in the investigative stage. A secondary result is that waveform distortions are duplicated in the model. A third effect is caused by the simultaneous dependence of the friction on Q and on the water surface elevation. This produces what has been called "tidal pumping." Note that in Equation (6.8) both Q and z are functions of time. If we assume that there is no steady flow (from river discharges) the time average of Q over a tidal cycle must be zero. However, positive values of Q (the flood tide) are correlated with larger values of z , and negative values of Q (the ebb) are associated with smaller values. Thus the average of S_e over a tidal cycle is non-zero, even in the absence of a steady flow component, whenever there is a progressive wave. (A standing wave, in which Q and z are 90 degrees out of phase, does not produce this effect.) Thus, the so-called mean half tide, i.e., the average water surface elevation, increases in the direction of travel of the wave. If the mean water surface elevation at two points is constrained to be equal, however, the result is that there is a net advection of flow in the direction of wave propagation. This effect of tidal pumping is simulated by analog models that incorporate the correct form of square-law friction.

1.2.3 An Analog Computer Element for Pollution Dispersion

The simplest type of diffusion equation with a convection term has the form

$$K \frac{\partial^2 \varphi}{\partial x^2} - u \frac{\partial \varphi}{\partial x} - \frac{\partial \varphi}{\partial t} = -f(x) \tag{6.9}$$

where φ is the concentration of a substance subject to diffusion and convection, u is the convective velocity, and x and t are the distance and time coordinates in a one-dimensional system. Furthermore, u is assumed independent of x, so that a single convective term with a derivative of φ with distance suffices. The term $-f(x)$ is the input of φ along the channel, which is assumed to be one-dimensional.

It will be assumed, as in analog modeling, that the distance along the channel is discretized, so that in developing the derivatives with respect to distance we must use finite differences. Time derivatives, on the other hand, remain continuous and infinitesimally defined. Let the subscripts 1, 2, and 3 refer to successive locations along the channel axis. Then the following approximations apply

$$\frac{\partial^2 \varphi}{\partial x^2} \approx \frac{1}{h^2} (\varphi_1 - 2\varphi_2 + \varphi_3) \tag{6.10}$$

$$\frac{\partial \varphi}{\partial x} \approx \frac{1}{2h} (\varphi_3 - \varphi_1) \tag{6.11}$$

where h is the distance spacing. We now solve for the value at location 2 in terms of values at adjacent locations. Inserting the finite-difference approximations into Equation (6.9), we have

$$\frac{K}{h^2} (\varphi_1 - 2\varphi_2 + \varphi_3) - \frac{u}{2h} (\varphi_3 - \varphi_1) = \frac{\partial \varphi_2}{\partial t} - f(x) \tag{6.12}$$

The integral form of Equation (6.12) is simpler to solve on analog computers:

$$\varphi_2 = \int \left[\left(\frac{K}{h^2} + \frac{u}{2h}\right) \varphi_1 + \left(\frac{K}{h^2} - \frac{u}{2h}\right) \varphi_3 - 2 \frac{K}{h^2} \varphi_2 + f(x) \right] dt \tag{6.13}$$

The block diagram for these operations is shown in Figure 6.2. Multiplication by a constant, here indicated by a rectangular box, is relatively simple. Additional operations of sign changing may be required if the multiplicative constants are negative. Depending on the signs of φ, the operations of summation and integration may be combined; this is often facilitated by associating the value of φ with alternative polarities of voltage at alternate nodes.

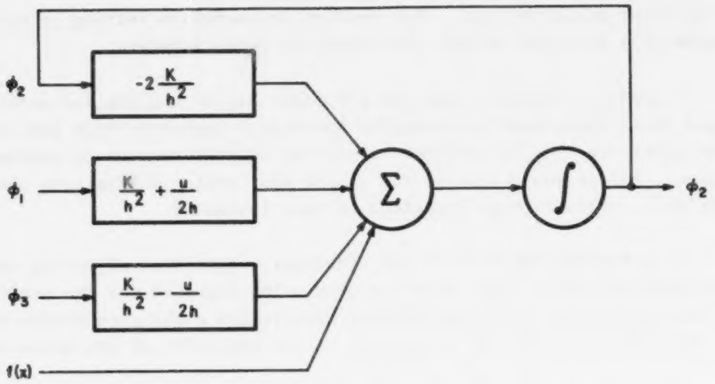

Fig. 6.2 Analog computation for Equation (6.13).

In this formulation, multiplication by a constant involves only a potentiometer setting, and one can see that by ganging three potentiometers the value of the constant K can be altered for all three inputs. If one separates positive and negative values of φ , a single setting can likewise alter the value of u through the use of double-gang potentiometers.

The simplest representation of a section of channel would require two sets of ganged potentiometers, two operational amplifiers (one each for sign inversion and integration) and one capacitor (as a part of the integrator). Inputs to the section would be an initializing setting (an electronic switch to a variable voltage source) to establish initial conditions for the integration, values for the constants K and u , and values of φ from adjacent nodes. In this formulation values of φ are related to voltages at the nodes and the computation is in terms of voltages in the usual way.

1.3 HYBRID COMPUTATION

Hybrid computers make use of both analog and digital computer elements. The analog section is used for the linear operations of integration, addition and subtraction. Since these operations can be carried out in parallel in most problems, a saving in computational time often results. The interface between the two sections is by means of analog-to-digital converters and digital-to-analog converters. Voltages from the analog section can be converted to a digital representation for use in the digital section, and digital output can be reconverted to voltages to serve as inputs to the analog section. In addition, the digital section can serve as a control for the analog through the use of servo-positioned potentiometers; in this way the digital section can alter scale factors. This feature is useful in setting up certain kinds of problems at a considerable increase in cost over hand-set potentiometers.

It appears, however, that the principal use of the digital section is the saving of results and their convenient recovery for subsequent insertion back into the analog section or subsequent print-out. It is possible to use the digital section to perform multiplications and table-lookups, but it would seem to the writer that analog multipliers and function generators could adequately perform these functions in most instances.

It is significant that in the practical application of analog computers to estuary dispersion problems there seems to be no convincing argument for the need for hybrid computing. However, the flexibility that some digital computation might give should not be entirely discounted; its usefulness will be a function of the ingenuity of the operator.

1.4 ECONOMIC CONSIDERATIONS IN ANALOG COMPUTING

Taking the basic operational amplifier as a measure of cost, prices may range from nearly $1,000 per unit down to as little as $20 per unit, or even less for some integrated circuit types. What one pays for in the highest priced units is long-term drift immunity, temperature stability, and the possibility of higher accuracy to a limit of about 0.01 percent. Less expensive units can be expected to perform at the 1.0 percent level, and may have to be used in a temperature-controlled environment to reduce drift. However, the provision of constant temperature cabinets is less of a problem considering the very compact nature of the small operational amplifier units. The smallest are no larger than a normal sized transistor in a TO-5 can.

Electronic multipliers are more expensive than amplifiers, but even here, if one is satisfied with 1 or 2 percent accuracy, integrated circuit versions can be bought for $25. The point is that the data usually available from pollution studies are rarely known with anything like one percent accuracy; and even if one takes into account that the cascading effect can increase the errors resulting from inaccurate components, it seems that the less expensive components would serve very well.

However, those firms that rent the use of analog computing equipment must ordinarily design their equipment for the most exacting of their customers, and this means expensive equipment and a correspondingly high rental figure. If it appears that the kinds of problems encountered in estuarine pollution studies can be profitably studied using analog computing equipment, one has two choices: rental of equipment, or purchase and in-house use of equipment. From a consideration of the accuracy requirements, it would seem that even a very large capacity analog computer could be assembled for no more cost than a nominal amount of rental of the high cost equipment normally available. The limitation would then be the skills of the personnel operating the equipment. However, high skill in this aspect of the operation is really necessary whether one rents or buys, for the rental firm cannot be expected to be experts in every field where their analog equipment is used.

It seems to the writer that under the assumption that analog equipment can be shown to be useful, an agency would be better advised to gather a small group of skilled operators and electronic experts, and let them have an in-house computer available to them all of the time. Very likely such an operation could handle all the problems in the U. S. and consist of a central laboratory facility.

1.5 SYSTEM-RESPONSE TYPE MODELS

If the water quality aspects of an estuary are considered to be a system in which inputs (in terms of nutrients, waste products, etc.) are related to outputs (such as BOD, algae levels), models can be constructed that do not make explicit assumptions about the physical processes that are taking place. This is often advantageous in those instances where we have little information about the actual processes.

A primitive form of such models is one in which one assumes a linear relationship between inputs and outputs; this is the same as assuming that each input acts independently of every other. This assumption is hardly realistic, but does offer the advantage that very simple mathematical techniques can be used. When one introduces the possibility of nonlinearity, the models become much more realistic, but the computational aspects become enormously complex, and tax the capabilities of even the largest computers. However, the trend towards ever faster and sophisticated computers will enable us to use system-response type models that are an ever more realistic means of understanding the process being modeled. The understanding, it must be emphasized, is in terms of predicting the response of the system to different levels and combinations of inputs, not in terms of understanding the actual physical processes themselves.

The feasibility of incorporating nonlinearity into systems analysis was advanced markedly by the work of Weiner (1958) and his colleagues at MIT (Bose 1956, Brilliant 1958, George 1959). Further work has been done by a group at the University of California in Berkeley (Amorocho 1961 and 1963, Jacoby 1962 and 1966). Recently Harder and Zand (1969) have brought the technique to a practical application. The general approach will be described in the following paragraphs.

In the process to be described, which has been called "the identification of nonlinear systems," the solution sought is the "system response function" by which an output function (usually a function of time) can be predicted from one or more input functions. In terms of water quality, the output function could be BOD at a particular location, algae population in a particular section of an estuary, etc. In one of the example problems examined by Harder and Zand (1969), the output function was the salinity at a certain location in an estuary, and the input function was the freshwater flow at the upper end of the estuary.

The system response function is obtained from an analysis of the past behavior of the system and is independent of any knowledge of the actual physical processes involved. Thus it does not use all the information available if the information includes such data as actual rates or processes, etc. On the other hand, it does not use any misinformation about what might be going on. It is a useful tool for predicting new behavior that is within the bounds of past behavior; it is not so reliable for extrapolating behavior.

The following explanation will use the example of salinity prediction as developed by Harder. The available input information was a record of freshwater inflow to the upper end of the San Francisco Bay estuary (Suisun Bay and the contiguous channels) over a period of ten years. This was discretized into averaged values for each one-third month period, giving 360 samples. Likewise, the salinity at Benicia (part way down the estuary) was discretized into a similar series of averaged values. Through a preliminary analysis it appeared that the "memory time" or the period after which the input influence on the output became negligible was about three months or nine periods. This meant that there were 351 (360 minus 9) sets of input variables; within each set there were nine sequential values of freshwater flow. Each of these sets was assumed to influence the value of salinity in the one-third month period immediately following the three-month period spanned by the set. Had a linear analysis been applied to this problem, nine weighting coefficients could have been attached to each of the nine input values preceding an output value (and distinguished by the lag time between each input value and the output value). Then a least-squares determination of these coefficients would lead to an equation from which the salinity (the output variable) could be predicted from a linear combination of the flows (the input variable) in the nine preceding periods. The error, while a minimum in the least-squares sense, is not the smallest that can be obtained.

Further reductions in the error of estimate can be obtained by including additional significant variables. In a nonlinear system these additional variables can be obtained by making use of squares and products of the original variables. In the present example, for instance, we could use nine squares and thirty-six distinguishable products, for a total of 54 linear and quadratic variables. This approach, while possible, is not necessarily the most efficient.

Harder and Zand (1969) made several improvements to this approach. First the input data sets were subjected to an orthogonal transformation so that the input values in each set could be represented more compactly; instead of nine values, perhaps six would be adequate. This transformation is linear, and tends to remove higher frequency components that might not be important. It has an additional function of allowing a weight factor to be introduced so that more distant (i.e., earlier) input variables can be given less weight than the more recent. The output of this linear economizing process is the input to the second stage in the analysis, the nonlinear process. Here products, squares, cubes, etc., are produced; these are called "super-variables" and are in turn entered into phase three, the stepwise linear regression processor. In this phase each of the super-variables is examined, and a determination is made of which one reduces the variance (between the measured and predicted output) the most. Provision is made at the present time (1970) to examine 74 variables at a time. At each succeeding step all the remaining variables are examined and the one which reduces the variance the most is included in the working set. At the same time, variables which have been included earlier are also examined, and those which became ineffective in reducing the error are dropped. The stepwise analysis continues until no addition or subtraction of a variable is effective in reducing the standard error of estimate by more than a stipulated minimum amount. At this point the associated super-variables and their coefficients are assembled into a predicting equation for use with new data. This mathematical construct constitutes the indentification of the system response function, and can be used to predict the response of the system to new input sequences.

In the Suisun Bay salinity analysis, the root-mean-square error between measured and predicted values was 15.9 percent. This figure included field measurement errors in both salinity and flows, and the error from ignoring other influences on the salinity such as evaporation, monthly variations in the mixing intensity as influenced by changing tide patterns, etc. As a check, a completely deterministic mathematical model of the estuary was constructed which exhibited approximately the same time constants and steady-state response as the real system. This artificial salinity system was then subject to the same input function as the real system (it was "forced" by the input function) and a "true" output obtained. The difference between the predicted output, from a system response analysis of the artificial system, and the "true" output constituted an error that could only be attributed to the analysis process itself. This error turned out to be 8.1 percent. By inference, were the various errors random and uncorrelated, the error in the real system that is not due to the analysis itself would be 13.7 percent.

In a second practical example in which two input functions were of importance, the inclusion of the second input, together with its interactions with the first, reduced the error from 7.4 percent to 4.4 percent.

In conclusion, it should be pointed out that system-response type models are in an active state of development and offer a promising new approach to certain kinds of water quality problems. Their further development should be encouraged.

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2. DIGITAL TECHNIQUES: FINITE DIFFERENCES

Jan J. Leendertse

2.1 INTRODUCTION

One of the most powerful methods in the integration of partial differential equations involves the replacement of the differential equation by one or more equivalent difference equations and solving the latter numerically. This approach has become increasingly more important with the growth in computation speed of computers and the increasing size of computer memories.

The difference equations used are approximations of the partial differential equations. Many different approximations can generally be made for each term of the partial differential equations, thus resulting in a wide selection. One would expect that one approximation might be better than another and this is generally true. The choice may also be governed, depending on the scope of the investigation, by the processes described by the equations, which may vary widely for the same equation. For example, in a computation of the tide in an estuary, we may select a scheme that places the emphasis on a good representation of tidal height in the area, while the mechanism of the dissipation of the wave energy by bottom friction, which in such cases is generally considerable, is not considered important. The scheme which we might use can even dissipate some energy just by the computation, and the rest of the dissipation is by some expressions in the finite-difference equations. Another scientist studying ocean circulation will be integrating the same long-wave equations, but is interested in the momentum transfer mechanism and the energy balance in the ocean. He will need a scheme that accurately describes the momentum fluxes, and in addition conserves energy. Another example is computation of the dispersion of pollutants. In working with rapidly decaying substances, a small decay by the computation may be acceptable, which would not be the case if the substance is conservative.

Not only have we to try to give the difference equation certain properties, we have to assure ourselves before all the effort is made to write a program, which may be the work of many years, that the computation can actually be made. In certain instances, the computation simply breaks down as errors start to grow and overshadow the solutions. Setting up and designing the computation requires considerable skill. The experienced worker in this field generally will be extremely careful in setting up his computation and will try to make predictions of the behavior of the computation. If certain detrimental effects do occur unexpectedly, he will try to trace the source of them and eliminate them, rather than arbitrarily make changes in the approximations. In the next sections, some of the methods which are used in these computations will be discussed.

From the above discussion it will be clear that the engineer or scientist who is in charge of an investigation must have experience in designing mathematical models and must know exactly the computational procedures used in order to assess the applicability and characteristics of the model which he uses in his investigation. As different approximations of the partial differential equations may lead to different representations of certain effects in the physical processes, the use of "box" or "cell" models is not advisable. The use of such models fixes immediately the finite-difference equations without regard to computational effects.

2.2 CONSIDERATIONS IN DESIGN OF COMPUTATION SCHEMES

2.2.1 Conservation of Mass

In a numerical computation, the mass in a bounded system should be conserved when account is made for the loss or gain of mass through the boundaries and for the sources and sinks in the system. For example, the continuity equation or the long-wave equation can be written

$$\frac{\partial \zeta}{\partial t} + \frac{\partial (Hu)}{\partial x} = 0 \tag{6.14}$$

where ζ = the distance between the water surface and the reference level,
H = temporal depth, the distance of the surface to the bottom, and
u = the velocity (averaged over the depth H).

Integration of Equation (6.14) in time and space between boundaries T_1, T_2, L_1, and L_2 yields zero.

$$\int_{L_1}^{L_2} \zeta \, dx \Big|_{T_1}^{T_2} + \int_{T_1}^{T_2} (Hu) \, dt \Big|_{L_1}^{L_2} = 0 \tag{6.15}$$

A difference scheme approximating Equation (6.14) and which satisfies the conservation of mass can be written, for example,

$$\begin{aligned} \zeta_m^{t+1} - \zeta_m^t + \frac{\Delta t}{\Delta x} \Big\{ & \left[h_{m+\frac{1}{2}} + \tfrac{1}{4}\left(\zeta_{m+1}^{t+1} + \zeta_{m+1}^{t} + \zeta_m^{t+1} + \zeta_m^t\right)\right] u_{m+\frac{1}{2}}^{t+\frac{1}{2}} \\ & - \left[h_{m-\frac{1}{2}} + \tfrac{1}{4}\left(\zeta_m^{t+1} + \zeta_m^t + \zeta_{m-1}^{t+1} + \zeta_{m-1}^t\right)\right] u_{m-\frac{1}{2}}^{t+\frac{1}{2}} \Big\} = 0 \end{aligned} \tag{6.16}$$

where ζ_m^t = water level at time t and at location $m\Delta x$,
h = depth from reference plane downward.

Numerical integration of (6.16) over one time step Δt for the range $m = 1$ to M results in

$$\begin{aligned} \Delta x \sum_{m=1}^{M} \zeta_m^{t+1} = \Delta x \sum_{m=1}^{M} \zeta_m^t + \Delta t \Big\{ & \left[h_{\frac{1}{2}} + \tfrac{1}{4}\left(\zeta_1^{t+1} + \zeta_1^t + \zeta_0^{t+1} + \zeta_0^t\right)\right] u_{\frac{1}{2}}^{t+\frac{1}{2}} \\ & - \left[h_{M+\frac{1}{2}} + \tfrac{1}{4}\left(\zeta_M^{t+1} + \zeta_M^t + \zeta_{M+1}^{t+1} + \zeta_{M+1}^t\right)\right] u_{M+\frac{1}{2}}^{t+\frac{1}{2}} \Big\} \end{aligned} \tag{6.17}$$

This shows that over one time step the mass is conserved; the latter two terms in the equation are the expressions for the inflow over the boundaries of the region. All other terms in the mass-fluxes cancel each other, even with varying velocity. (Equation (6.16) is difficult to solve because of the quadratic terms, and has been used here only as an example.)

It will be noted that Equation (6.14) can also be written

$$\frac{\partial \zeta}{\partial t} + H \frac{\partial u}{\partial x} + u \frac{\partial \zeta}{\partial x} = 0$$

With this representation it is very difficult to set up a difference scheme such that the numerical integration cancels all the finite-difference approximations of the fluxes in the field between the boundaries.

From a careful analysis of the finite-difference equations, an experienced engineer or scientist will rather rapidly determine if the conservation laws are satisfied. Sometimes an experimental investigation has to be made. For example in a tidal computation, the variation of the balance of the content of the bay minus the inflow over a tidal cycle should be small compared to the tidal prism. In an advective and diffusive transport computation which is coupled to such a tidal computation, a computation of the mass balance of a conservative substance should be performed. In addition, a computation should be made with constant mass concentrations as initial conditions and the same constant mass concentration on the boundaries. All values in the whole system should stay constant during computation over a tidal cycle.

2.2.2 Stability

In the finite-difference equations employed for approximating the differential equations, it is also required that numerical errors introduced in the computation do not amplify in an unlimited manner.

One approach toward the investigation of stability (O'Brien *et al*. 1950) is to follow a Fourier expansion of a line of errors as time progresses. Let us assume to have a finite-difference approximation

$$C_m^{t+1} - C_m^t + \frac{1}{2} \frac{\Delta t}{\Delta x} u(C_{m+1}^t - C_{m-1}^t) - \frac{\Delta t}{(\Delta x)^2} D_x(C_{m+1}^t - 2C_m^t + C_{m-1}^t) = 0 \qquad (6.18)$$

Suppose that a line of errors $\delta C(x)$ exists at a particular time t, which we set conveniently at $t = 0$. It is possible to make a finite Fourier decomposition of these errors as follows:

$$\delta C(x) = \sum_n A_n e^{i\sigma_n x} \qquad (6.19)$$

In our computation a finite number of points N exists in the x direction and the number of terms n of this decomposition equals N.

We consider u to be constant, so that a linear system is being considered. Consequently, the behavior of only one term of the Fourier series needs to be followed. The components A_n are time-dependent, and, in order to satisfy the expression of the particular error wave at $t = 0$, the components must take the form

$$A_n = \bar{a}_n e^{i\beta_n t} \tag{6.20}$$

where $\bar{a}_n$ and β_n are constants. Thus the expressions for the errors at (t,x) of the mass concentration C should satisfy the form

$$\delta C(x,t) = \bar{a}_n e^{i\beta_n t} e^{i\sigma x} \tag{6.21}$$

It is assumed that the errors are perturbations imposed upon the solutions of the linear system. If we subtract the exact solutions from the solutions of the difference equations with the perturbations, we obtain among the error components a set of relations that are identical to the relations for the components of C, as we are dealing with a linear system. Introducing Equation (6.21) into the set of equations which represent the relation of the errors and using only values of x and t on the grid results in relations between β and σ.

Using $\lambda = e^{i\beta\Delta t}$ then

$$(\lambda - 1)\bar{a} + u \frac{\Delta t}{2\Delta x}(e^{i\sigma\Delta x} - e^{-i\sigma\Delta x})\bar{a} - D_x \frac{\Delta t}{(\Delta x)^2}(e^{i\sigma\Delta x} - 2 + e^{-i\sigma\Delta x})\bar{a} = 0 \tag{6.22}$$

from which we find for nontrivial solutions

$$\lambda = 1 - iu \frac{\Delta t}{\Delta x} \sin(\sigma\Delta x) - 4 \frac{\Delta t\, D_x}{(\Delta x)^2} \sin^2(\sigma\Delta x/2) \tag{6.23}$$

In order that the original error, with components $A_n e^{i\sigma_n x}$, shall not grow as t increases, it is necessary that

$$|e^{i\beta_n \Delta t}| \leq 1 \tag{6.24}$$

Thus, it is necessary for stability that

$$|\lambda| \leq 1 \tag{6.25}$$

Therefore from Equation (6.23) and Equation (6.25) we can derive the condition which is necessary for stability. For example if $u = 0$, then

$$\frac{\Delta t}{(\Delta x)^2} D_x < \frac{1}{2}$$

Even for this simple linear case, the derivation of the necessary conditions for stability is a considerable task, and it becomes increasingly more difficult if systems of equations are involved, such as the long-wave equations in two directions. In the latter case, necessary conditions for stability are found by a similar process as described above, but now with vectors and matrices, and the stability condition will finally be derived from the eigenvalues of the so-called amplification matrix. In the simple case (Equation 6.18), the amplification matrix has only one component, which is its eigenvalue λ.

Up to this time we have concerned ourselves only with linear equations and it may be noted that in the discussions the conditions we have derived are conditions necessary for stability. Conditions which are also sufficient for stability are much more difficult to obtain (see Richtmyer and Morton 1967).

One particularly troublesome phenomenon is the generation of nonlinear instability. The analysis described above is applicable for linear systems. In fluid flow computations, this is generally never the case; the equations are nonlinear or have variable coefficients. If we have a term of the type $u \, \partial u/\partial x$ in a two-dimensional system, the velocities are sums of Fourier terms

$$u^* \cos(\sigma_{1_m} x + \sigma_{2_m} y)$$

The expression $u \, \partial u/\partial x$ then yields expressions with sums and differences of wave numbers σ_1 and σ_2 which results in wavelengths associated with these wave numbers that are smaller than the grid size of our computation. The computation aliases these waves to larger ones, and a rapid growth of fluctuations with short wavelength is the result. The easiest way to eliminate this is the introduction of artificial viscosity or dispersion, but from the previous discussions it is clear that the whole computation can become meaningless. If such an approach is taken, a very careful analysis of this effect has to be made. Some computational schemes have a built-in dissipative effect which we can find by the analysis in Section 2.2.4. The more elegant methods of the elimination of nonlinear feedback are by "filtering" the short wavelength in the nonlinear term. For example, Equation (6.16) eliminates feedback of wavelength $2\Delta x$ in the water levels.

The expressions for these nonlinear terms have become very sophisticated in solutions of other fluid dynamics problems, as conservation can be obtained of quadratic properties such as energy and vorticity. For discussion of the stability of such schemes, the reader is referred to Lilly (1965) and Grammeltvedt (1969).

Boundary conditions can also introduce instabilities. For example, in tidal computations a velocity is sometimes represented as a function of water level, such as occurs in submerged barriers. The relation which we may unknowingly impose is a condition that gives solutions of the type $e^{\sigma x}$, which are then generated as a computational mode. This phenomenon has been observed by Reid and Bodine (1968) and Masch *et al.* (1969) for submerged barriers, and by Leendertse (1970) in the computation of moving boundaries across tidal flats in two-dimensional tidal computations.

2.2.3 Dissipative and Dispersive Effects

Periodic fluctuations which we are representing with finite-difference schemes deviate generally from the analytic solutions, as we are using finite-difference equations and thus are making approximations. These effects can be *dissipative* and *dispersive*. "Dissipative" means that periodic fluctuations in the spatial field are decreased in time by the computations. "Dispersive" means that the propagation speed differs from the analytic speed in a manner which is dependent on the wavelength. Suppose, in an estuary with a constant current, a certain distribution of a conservative substance exists. This distribution can be thought to consist of a summation of periodic fluctuations in the spatial dimension. Dissipative effects of the computation will diminish the amplitude of these fluctuations, and the dispersive effects will change the shape of the distribution by the differences in the speed of propagation in the computation. The field becomes deformed; the fluctuations with shorter wavelengths are generally overtaken by those with larger wavelengths.

As an example, the one-dimensional advective transportion equation will be used,

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} - D_x \frac{\partial^2 C}{\partial x^2} = 0 \tag{6.26}$$

for which we now use the approximation

$$C_m^{t+1} - C_m^t + u\,\frac{\Delta t}{2\Delta x}\left(C_{m+1}^{t+1} - C_{m-1}^{t+1}\right) - D_x\,\frac{\Delta t}{\Delta x^2}\left(C_{m+1}^{t+1} - 2C_m^{t+1} + C_{m-1}^{t+1}\right) = 0 \tag{6.27}$$

Following the derivation in Section 2.2.2, we obtain the eigenvalue

$$\lambda = 1/\left[1 + \frac{\Delta t}{\Delta x} iu\,\sin(\sigma\Delta x) + 4D_x\,\sin^2(\sigma\Delta x/2)\cdot\frac{\Delta t}{(\Delta x)^2}\right] \tag{6.28}$$

It can be expected that computation with this scheme will meet no difficulty. The absolute value of the eigenvalue is smaller than unity, thus the necessary condition is met and the computation is stable, assuming u is a constant. Any spatial fluctuation or wave will decay in amplitude. This fact is also true if the dispersion or diffusion coefficient is zero. In the latter case, the computation introduces dissipation and this dissipation is dependent on the time step, the spatial grid size, the velocity, and the wave number σ. The fluctuations with short wavelengths are particularly affected, and this computation acts as a filter on such short waves.

The dispersive effect can be investigated also by use of the eigenvalues. To illustrate this effect again the assumption is made that the dispersion coefficient in Equation (6.26) is zero. The propagation speed of the Fourier components is naturally the velocity u. The following relation between frequency and wave number exists:

$$\omega/\sigma = u \tag{6.29}$$

For the finite-difference equation (6.27) we find, following the explanation in Section 2.2.2, for the eigenvalue

$$\lambda = e^{i\omega'\Delta t} = 1/\left(1 + \frac{\Delta t}{\Delta x} iu\,\sin(\sigma\Delta x) + 4\,\frac{D_x\Delta t}{(\Delta x)^2}\,\sin^2(\sigma\Delta x/2)\right) \tag{6.30}$$

where ω' = frequency of the computational system. As an eigenvalue smaller than unity was obtained, this frequency ω' is a complex number, of which the imaginary part is related to the dissipative effect. If we set

$$A = \frac{\Delta t}{\Delta x} u\,\sin(\sigma\Delta x) \tag{6.31}$$

then for $D_x = 0$, Equation (6.30) can be written

$$e^{i\omega'\Delta t} = (1 - iA)/(1 + A^2) \tag{6.32}$$

from which we find for the real part

$$\mathrm{Re}[\omega'\Delta t] = \tan^{-1}(A) \tag{6.33}$$

With an expansion for the inverse trigonometric function, this becomes

$$\omega'\Delta t = A - \frac{1}{3}A^3 + \frac{1}{5}A^5 \ . \ . \ . \tag{6.34}$$

or

$$\omega'\Delta t = \frac{\Delta t}{\Delta x}\, u \sin(\sigma\Delta x) \left[1 - \frac{1}{3}A^2 + \frac{1}{5}A^4 - . \ . \ . \right] \tag{6.35}$$

and by also replacing sin(σΔx) by its power series then

$$\frac{\omega'}{\sigma} = u\left[1 - \frac{(\sigma\Delta x)^2}{3!} + \frac{(\sigma\Delta x)^4}{4!} - . \ . \ . \right]\left[1 - \frac{1}{3}A^2 + \frac{1}{5}A^4 - . \ . \ . \right] \tag{6.36}$$

Both series are smaller than unity. Thus for all values of $\Delta t\, u/\Delta x$, the computed wave propagates slower than the analytic solution. When $\Delta x \to 0$ and $\Delta t \to 0$ both series approach unity and, as we would expect, the computed wave speed converges to the speed of the analytic solution, as shown in Figure 6.3. It will be noted that when the representation is on a grid with less than ten points per wavelength, the representation becomes very poor. The representation in the spatial dimension is more important than the discreteness in time.

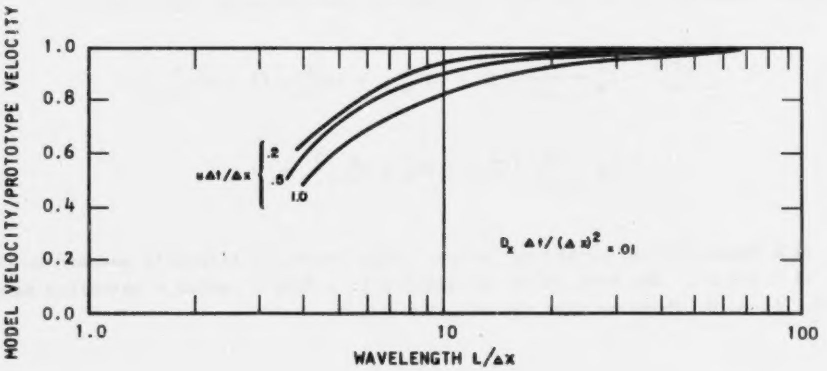

Fig. 6.3 Ratio of the velocity in the model and velocity in prototype as function of the spatial representation.

In the analysis of a computational scheme, the dissipative effects can be expressed as the ratio of the amplitude of the computed solution and the amplitude of the theoretical solution after the time interval that the Fourier component travels over its wavelength. For Equation (6.26) and $D_x = 0$, the amplitude of any component of the analytic solution stays the same. For the computation using (6.27) with each time step, the amplitude decreases according to the absolute value of λ.

For the time step Δt, the number of times that we have to compute for the time interval that the analytical solution propagates over its wavelength is

$$n = \frac{L}{u\Delta t} = 2\pi/u\Delta t\sigma \tag{6.37}$$

The ratio of the amplitudes becomes

$$|T(\sigma\Delta x)| = \left[1/\sqrt{1 + A^2}\right]^n \tag{6.38}$$

This ratio is called the modulus of the propagation factor (Leendertse 1967). By plotting this modulus as a function of the number of points per wavelength, a clear insight is obtained into the filtering effects of the computational schemes.

The dissipative and dispersive effects also manifest themselves in tidal computations. The physical process in itself generally is rather strongly dissipative by the bottom frictions, which then are used to adjust tidal heights in the verification of the model. With a coarse grid, the higher frequencies in the tidal curves are generally dampened or disappear, and the phase of the tidal curves cannot be matched.

2.2.4 Effects of Noncentered Operations

For conceptual reasons (Thomann 1963) or for reasons of stability, the advective term is sometimes taken noncentered in space. Again, this will be studied using the linear advective transport equation (6.26) for which we now use the following approximation

$$\begin{aligned} C_m^{t+1} - C_m^t + \frac{\Delta t}{2\Delta x} u\left[(1+\alpha)C_{m+1}^t - 2\alpha C_m^t - (1-\alpha)C_{m-1}^t\right] \\ - D_x \frac{\Delta t}{(\Delta x)^2}\left[C_{m+1}^t - 2C_m^t + C_{m-1}^t\right] = 0 \end{aligned} \tag{6.39}$$

where α is a dimensionless weighting factor. This factor is generally assumed to be in the range of $-1 < \alpha < 1$. The form (6.39) is similar to a form in which a so-called advection factor (ξ) is used, where we have the relation

$$\xi = \frac{1}{2} + \frac{1}{2}\alpha$$

Equation (6.39) can also be written

$$C_m^{t+1} - C_m^t + \frac{\Delta t}{2\Delta x} u\left[C_{m+1}^t - C_{m-1}^t\right]$$

$$- \left(D_x - \tfrac{1}{2}\alpha\Delta x u\right) \frac{\Delta t}{(\Delta x)^2}\left(C_{m+1}^t - 2C_m^t + C_{m-1}^t\right) = 0$$

It will be clear that the off-centered differencing is in effect an increase or decrease of the dispersion coefficient. Following the LeLevier method, as described by Richtmyer and Morton (1967), so-called "upstream" differencing results in an increase of stability of the computation and an effective increase of the dispersion coefficient. Such upstream differencing uses, then, the values for α ,

$$\alpha < 0 \quad \text{if } u > 0$$

$$\alpha > 0 \quad \text{if } u < 0$$

The artificial dispersion introduced in this manner makes the actual values of the dispersion coefficients used meaningless if we do not account for these effects. Dispersion coefficients are generally found by trial and error until observed values match the computed values. The use of off-centered operations will now make the apparent dispersion coefficient a function of the grid size.

The forward implicit scheme (Equation 6.27) which has been discussed previously, showed considerable artificial dispersion caused by the noncentered forward stepping. It was shown also that the forward-stepping scheme (explicit) showed just the opposite, as for small wavelengths the system becomes unstable. In other words, the dispersion term is not able to diminish some components.

In view of this, it can be expected that the alternating use of the explicit and implicit scheme might lead to better results, and this can easily be derived from above discussions. In this manner multioperation schemes are formed, in which two (or more) approximations are used for one partial differential equation. Since implicit schemes are often difficult to solve, particularly if several spatial dimensions are present, a multioperation approach will give flexibility in computations, as spatial gradients can be taken alternatingly in the forward and backward fashion. The equations become, then, implicit in one dimension only.

2.2.5 Discontinuities

Considerable difficulties are encountered if the system, which we represent by finite-difference equations, has discontinuities. At such discontinuities the Fourier decomposition will present large contributions of very short wavelength, which we are not able to represent. One of the most frequently used ways, first used by Von Neumann (see Richtmyer and Morton 1967), is to introduce artificial viscocity or dispersion at the location of the discontinuity, thus locally smoothing the solution. An expedient way is to use local upstream differencing. For example, for the advective transport equation with a source at location m , the finite-difference expression becomes

$$C_m^{t+1} - C_m^t + \frac{\Delta t}{2\Delta x} u\left(C_{m+1}^{t+1} + C_m^{t+1} - 2C_{m-1}^{t+1}\right)$$

$$+ \frac{\Delta t D_x}{(\Delta x)^2}\left(C_{m+1}^{t+1} - 2C_m^{t+1} - C_{m-1}^{t+1}\right) + S_m \Delta t = 0 \qquad (6.40)$$

if $u > 0$, where S_m is the contribution of the source per time interval. To conserve mass, the equation which is upstream of the point m , in this case at $m - 1$, has been written

$$C_{m-1}^{t+1} - C_{m-1}^t + \frac{\Delta t}{2\Delta x} u\left(2C_{m-1}^{t+1} - C_{m-1}^{t+1} - C_{m-2}^{t+1}\right)$$

$$+ \frac{\Delta t D_x}{(\Delta x)^2}\left(C_m^{t+1} - 2C_{m-1}^{t+1} + C_{m-2}^{t+1}\right) + S_{m-1}\Delta t = 0 \qquad (6.41)$$

With this approach, the influence of the source at location m is not felt upstream other than through the contribution of the dispersion term. If the normal finite-difference equation is used at the source, the upstream point generally becomes severely suppressed, and in actual computations a dampened spatial oscillation appears.

A more elegant method than the one described above is the introduction of artificial dissipation in such a form that the contribution is negligible if the adjacent concentration values are nearly equal, but is the required additional dispersive effect if adjacent values are widely different (Richtmyer and Morton 1967). For example, the disperson coefficient $m + \frac{1}{2}$ can be expressed

$$D_{m+\frac{1}{2}} = D\left[1 + \frac{\left(c_{m+1}^t - c_m^t\right)^2}{\left(c_{m+1}^t + c_m^t\right)^2} \cdot K\right]$$

where K is a constant, which has to be determined experimentally.

2.2.6 Comments on Higher Order Schemes

In mathematical modeling, the spatial representation or discreteness is often a limiting factor, particularly in two-dimensional computations, as large arrays have to be kept in active memory of the computer. First the representation of depth or volume is generally somewhat inaccurate as hydrographic surveys present only data in lines through the area, and secondly the finite-difference approximations which are used give a rough approximation. Consequently, higher order approximations in the spatial dimension seldom give a noticeable increase in accuracy.

For the time integration, higher order schemes have been used, for example the solution of the one-dimensional long-wave equation by Collins and Fersht (1968), and the solution by Jeglic (1966) of the advective and diffusive transport of pollution constituents of the model by Thomann (1963). Both Collins and Fersht (1968) and Jeglic (1966) use a Runge-Kutta equation. Very high accuracy can be obtained with this method for the solution of ordinary differential equations. This is not the case for the solution of partial differential equations.

The time-stepping procedure uses higher order derivatives in time and space. For example, in the first mentioned scheme, in the time step of the transport Q in the momentum equation, a fourth-order spatial derivative of Q is used. On the other hand, in the equation of continuity the spatial representation of $\partial Q/\partial x$ has only a third-order accuracy. A Taylor series expansion of the finite-difference approximation will show that such fourth-order spatial derivatives are truncated! Consequently these methods have then only an apparent high accuracy. The time step is noncentered and introduces a dissipative effect, which offsets the inherent instability of the forward-stepping scheme, such as the one analysed in Section 2.2.2. As direct forward-stepping methods which are centered in time are available, a much more efficient computation can now be achieved with the same or better accuracy.

2.2.7 Use of Conservation Laws to Obtain Nonlinear Stability

In Section 2.2.2 it was indicated that the nonlinear terms or term with variable coefficients have a tendency to introduce nonlinear instabilities. The conservation law can be used for the design of schemes such that these instabilities are suppressed without making the computation strongly dissipative. The principle upon which schemes are designed will be illustrated by use of the advection equation

$$\frac{\partial c}{\partial t} + \frac{\partial (uc)}{\partial x} = 0 \qquad (6.42)$$

The diffusion term which normally appears in the computation of water quality characteristics has been omitted as it would make the discussion more complicated. Let us now consider that the region of computation is bounded and has no inflow, which then reduces our problem to concentration distributions in a closed-off channel in which the substances are moved advectively by nonsteady currents.

If we apply the conservation law to the mass conservation of the substance c, as described in 2.2.1, the total mass does not change. For example, in Figure 6.4a, the area under the solid line, representing the total mass at time t_1, is equal to the area under the dashed curve at time t_2, as

$$\int_{\ell_1}^{\ell_2} c \, dx = \text{constant}$$

which means that the first statistical moment of the variable c is conserved, or, in other words, the mean value of c is conserved. In numerical computation, it is generally imperative that this law be satisfied in order to obtain meaningful results. In numerical computation, the area of integration bounded by sectional lines over distances Δx should stay constant after computation over a certain number of time steps (Figure 6.4b). This does not guarantee that the computation has stability; the results may show a typical instability and still satisfy the conservation law of the mass of the substance (Figure 6.4c).

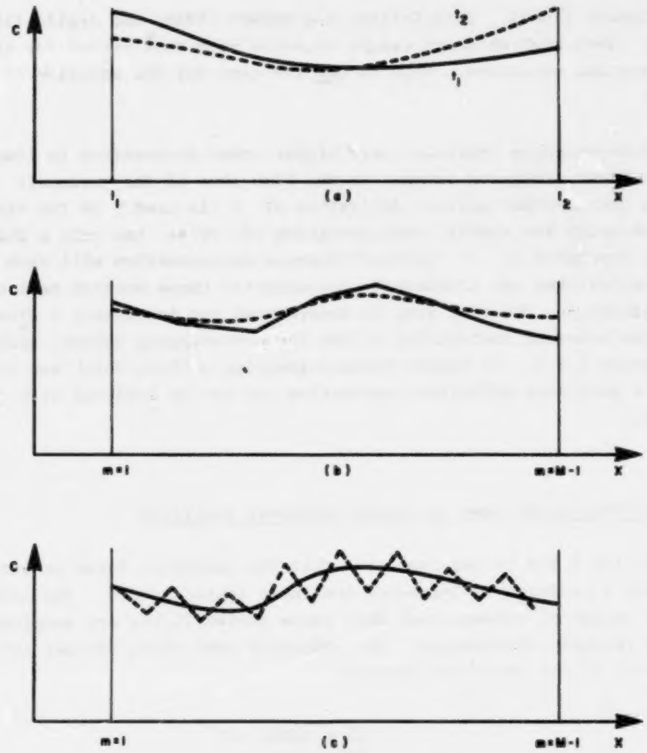

Fig. 6.4 Spatial concentration profiles for successive time levels exhibiting conservation of mass (see text).

To design a nonlinear stable scheme, one can also conserve, in addition to the first statistical moment of the variable c, the second statistical moment of the variable, or, in other words, conserve the mean variance. If Equation (6.42) is multiplied by c and integrated over the region from ℓ_1 to ℓ_2 with closed boundaries, we obtain

$$\int_{\ell_1}^{\ell_2} c \frac{\partial c}{\partial t} dx + \int_{\ell_1}^{\ell_2} c \frac{\partial (uc)}{\partial x} dx = 0 \qquad (6.43)$$

This equation can also be written

$$\frac{1}{2} \frac{\partial \int c^2 dx}{\partial t} + \frac{1}{2} \int c^2 \frac{\partial u}{\partial x} dx + \frac{1}{2} \int \frac{\partial (uc^2)}{\partial x} dx = 0 \qquad (6.44)$$

As no inflows at the boundaries are assumed, the third term becomes zero and Equation (6.44) reduces to

$$\frac{1}{2}\,\frac{\partial\int c^2 dx}{\partial t} + \frac{1}{2}\int c^2\,\frac{\partial u}{\partial x}\,dx = 0 \tag{6.45}$$

Thus, the finite-difference scheme has to satisfy also Equation (6.45). By imposing this restriction, the number of schemes which are now available is severely reduced, and solutions are obtained which cannot obtain the pattern shown in Figure 6.4c.

A finite-difference approximation of Equation (6.42) can be written

$$\begin{aligned}&\left(c_m^{t+1} - c_m^t\right)/\Delta t + \Big[\left(c_{m+1}^{t+1} + c_{m+1}^t + c_m^{t+1} + c_m^t\right)\left(u_{m+\frac{1}{2}}^{t+1} + u_{m+\frac{1}{2}}^t\right)\\ &- \left(c_m^{t+1} + c_m^t + c_{m-1}^{t+1} + c_{m-1}^t\right)\left(u_{m-\frac{1}{2}}^{t+1} + u_{m-\frac{1}{2}}^t\right)\Big]/8\Delta x = 0\end{aligned} \tag{6.46}$$

Following Section 2.2.1, it can be seen that numerical integration over one time step Δt for the range $m = 1$ to $m = M$, with $u_{\frac{1}{2}}^t = u_{\frac{1}{2}}^{t+1} = u_{M-\frac{1}{2}}^t = u_{M-\frac{1}{2}}^{t+1} = 0$, results in

$$\sum_{m=1}^{M} c_m^{t+1} - \sum_{m=1}^{M} c_m^t = 0 \tag{6.47}$$

The conservative property of the variance of c in Equation (6.46) can be demonstrated by multiplying both sides of Equation (6.46) by

$$\frac{1}{2}\left(c_m^{t+1} + c_m^t\right) \tag{6.48}$$

after which we find

$$\begin{aligned}&\frac{1}{2}\left(c_m^{t+1} + c_m^t\right)\cdot\left(c_m^{t+1} - c_m^t\right)/\Delta t\\ &+ \left(c_m^{t+1} + c_m^t\right)^2\left(u_{m+\frac{1}{2}}^{t+1} + u_{m+\frac{1}{2}}^t - u_{m-\frac{1}{2}}^{t+1} - u_{m-\frac{1}{2}}^t\right)/16\Delta x\\ &+ \left(c_m^{t+1} + c_m^t\right)\left(c_{m+1}^{t+1} + c_{m+1}^t\right)\left(u_{m+\frac{1}{2}}^{t+1} + u_{m+\frac{1}{2}}^t\right)/16\Delta x\\ &- \left(c_{m-1}^{t+1} + c_{m-1}^t\right)\left(c_m^{t+1} + c_m^t\right)\left(u_{m-\frac{1}{2}}^{t+1} + u_{m-\frac{1}{2}}^t\right)/16\Delta x = 0\end{aligned} \tag{6.49}$$

For the summation of all points in the field we find from (6.49)

$$0 = \frac{1}{2\Delta t}\sum_{m=1}^{M}\left\{\left(c_m^{t+1}\right)^2 - \left(c_m^{t}\right)^2\right\}$$

$$+ \frac{1}{16\Delta x}\sum_{m=1}^{M}\left(c_m^{t+1} + c_m^{t}\right)^2\left\{\left(u_{m+\frac{1}{2}}^{t+1} + u_{m+\frac{1}{2}}^{t}\right) - \left(u_{m-\frac{1}{2}}^{t+1} + u_{m-\frac{1}{2}}^{t}\right)\right\} \qquad (6.50)$$

Note that the last two terms of (6.49) are cancelled in the summation by the contributions of the adjacent points. Equation (6.50) represents a finite-difference form which is analogous to the integrated differential equation (6.45).

2.3 TIDAL COMPUTATIONS

2.3.1 One-Dimensional Computations

An extensive literature exists concerning one-dimensional computations. A review of these methods is given by Dronkers (1964, 1969). Of particular importance to water quality modeling is the expression for the continuity equation

$$\frac{\partial Q}{\partial x} + b\,\frac{\partial \xi}{\partial t} = 0 \qquad (6.51)$$

where Q denotes the discharge through a cross section, b the width and ξ distance of water level to reference plane. In this formulation, it is assumed that the fluid density is constant. If the tidal computation is used in conjunction with water quality computation, both computations should be compatible. This will be discussed under water quality modeling. Most one-dimensional tidal computations have not been designed especially for water quality modeling, consequently their applicability should be analyzed carefully, particularly as to the conservation of mass.

In computations of estuaries, considerable difficulties are generally experienced in estuary networks. There is a tendency to use an explicit computation, where all new values at $t + \Delta t$ can be obtained directly from previous information, but stability limits on the time step makes such computations of a long duration. Dronkers (1969) indicated an implicit scheme for an upward branching network. A multioperation method can be very useful in such cases. One operation is then explicit, the second implicit (Leendertse 1967). With careful layout, one part of the system is computed with the explicit step, the other part implicit. With the next operation, the first-mentioned part is computed implicit and the second part now explicit.

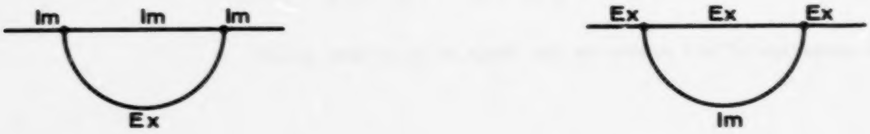

Fig. 6.5 Diagrammatic representation of multioperation technique.

Computation of the implicit part is relatively fast by use of a sweep method (Leendertse 1967, Dronkers 1969). This method has no limit for stability reasons on the time step.

2.3.2 Two-Dimensional Tidal Computations

The partial differential equations used for estuaries with vertical homogeneity are a set of equations with velocity components and water level as the dependent variables (see Chapter II, Section 2, Dronkers 1969, Hansen 1962, Leendertse 1967).

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} + g\frac{\partial \xi}{\partial x} - fv + R(x) = F(x) \qquad (6.52)$$

$$\frac{\partial v}{\partial t} + u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y} + g\frac{\partial \xi}{\partial y} + fu + R(y) = F(y) \qquad (6.53)$$

$$\frac{\partial \xi}{\partial x} + \frac{\partial[(h+\xi)u]}{\partial x} + \frac{\partial[(h+\xi)v]}{\partial y} + S = 0 \qquad (6.54)$$

The velocity components u and v are averaged in the vertical, and

f = Coriolis parameter,

$R(x)$, $R(y)$ = expressions for bottom friction

$F(x)$, $F(y)$ = forcing functions by wind and barometric pressure differences

Rather than the vertical-averaged velocity components, some investigators use as the variable the transport over a section with unit width (Reid and Bodine 1968, Masch et al. 1969).

$$\frac{\partial Q_x}{\partial t} - fQ_y + \frac{\partial(Q_x^2/H)}{\partial x} + \frac{\partial(Q_xQ_y/H)}{\partial y} + g\,H\frac{\partial \xi}{\partial x} + R(x) = F(x) \qquad (6.55)$$

$$\frac{\partial Q_y}{\partial t} + fQ_x + \frac{\partial(Q_xQ_y/H)}{\partial x} + \frac{\partial(Q_y^2/H)}{\partial y} + g\,H\frac{\partial \xi}{\partial y} + R(y) = F(y) \qquad (6.56)$$

$$\frac{\partial \xi}{\partial t} + \frac{\partial Q_x}{\partial x} + \frac{\partial Q_y}{\partial y} + S = 0 \qquad (6.57)$$

where Q_x and Q_y are the components of transport per unit width. Masch et al. (1969) omit the convective terms, which are relatively unimportant in his investigation.

The finite-difference approximations for each of the two sets generally use a network of the type shown in Figure 6.6. Computation is very favorable, as for each point at which the computation is advanced in time (for example u in Equation 6.52), the spatial gradient of the other important variable (ξ in Equation 6.5.2) is present centered in space. Gates (1968), integrating the long-wave equations for an investigation of ocean circulation, has an additional network, of the type shown in Figure 6.6, which is located with shifted coordinates over distances half the grid size in both directions x and y . In the grid scheme, both components of the velocity are available at the same location.

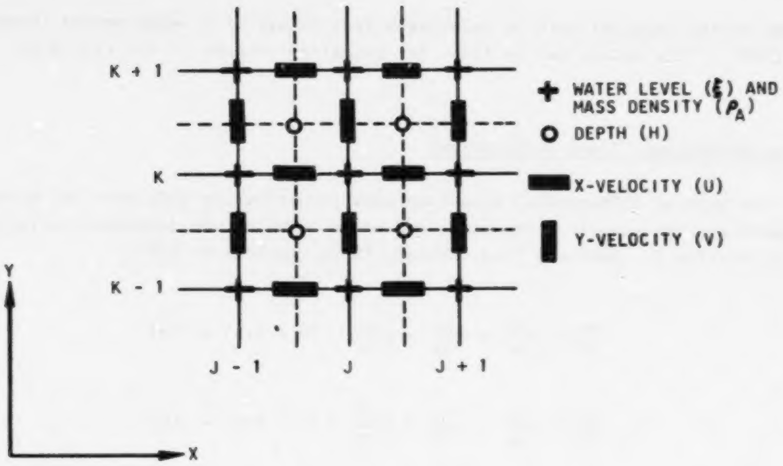

Fig. 6.6 Example of space-staggered scheme.

The time operations which are presently most widely used in two-dimensional computations are either of the so-called "leap frog" type, or are an implicit multioperation method. Both methods are time-centered difference schemes for the main terms in the equations. For discussing these stepping methods, the partial differential equations (6.55) through (6.57) are now written

$$\frac{\partial Q_x}{\partial t} + F_1 + F_2 = 0 \tag{6.58}$$

$$\frac{\partial Q_y}{\partial t} + G_1 + G_2 = 0 \tag{6.59}$$

$$\frac{\partial \xi}{\partial t} + H_1 + H_2 = 0 \tag{6.60}$$

The terms F_1 , F_2 , F_3 represent the remaining group of terms in Equations (6.55) through (6.57). For example, we can take

$$F_1 = g\,H\frac{\partial \xi}{\partial x} \tag{6.61}$$

and

$$F_2 = \frac{\partial(Q_x^2/H)}{\partial x} + \frac{\partial(Q_xQ_y/H)}{\partial y} - fQ_y + R(x) - F(x) \tag{6.62}$$

In the leap frog computations are used the finite-difference equations

$$Q_x^{t+\Delta t} - Q_x^{t-\Delta t} = -2\ \Delta t\ F_1^t \tag{6.63}$$

$$Q_y^{t+\Delta t} - Q_y^{t-\Delta t} = -2\ \Delta t\ G_1^t \tag{6.64}$$

$$\xi^{t+\Delta t} - \xi^{t-\Delta t} = -2\ \Delta t\ H^t \tag{6.65}$$

where F_1^t , G_1^t , and H^t are the finite-difference expressions for all other terms of Equations (6.55) through (6.57). For example, F_1^t now represents the finite-difference expression at time t for

$$g\ H\frac{\partial \xi}{\partial x} + \frac{\partial (Q_x^2/H)}{\partial x} + \frac{\partial (Q_x Q_y/H)}{\partial y} - fQ_y + R_x - F(x) \tag{6.66}$$

This scheme has a high accuracy but requires two levels of storage of all values Q_x , Q_y and ξ , namely at time t and time $t-\Delta t$. Such a computation is made by Gates (1968). To reduce this storage requirement, time-staggered computations are made with Q_x and Q_y at the odd time levels $(t-1)$ and the water levels at the even time levels t . Such computations are made by Hansen (1962) and Masch (1969). (Masch indicates, in the time notations, that the water levels are at the same level as the transports, but a careful review will reveal that they are always taken at the intermediate level, namely centered in time.)

For the computations of the latter, we obtain, neglecting bottom friction in our discussion,

$$Q_x^{t+1} - Q_x^{t-1} = 2\ \Delta t\ (F_1^t + F_2^{t-1}) \tag{6.67}$$

$$Q_y^{t+1} - Q_y^{t-1} = 2\ \Delta t\ (G_1^t + G_2^{t-1}) \tag{6.68}$$

$$\xi^{t+2} - \xi^t = 2\ \Delta t\ H_1^{t+1}$$

where $F_1^t \doteq -g\ H\frac{\partial \xi}{\partial x}$ at time t ('$\doteq$' means 'is the finite-difference representation of')

$F_2^{t-1} \doteq fQ_y - F(x)$ at time t-1,

$G_1^t \doteq -g\ H\frac{\partial \xi}{\partial y}$ at time t,

$G_2^{t-1} \doteq fQ_x - F(y)$ at time t-1, and

$H^{t+1} \doteq \frac{\partial Q_x}{\partial x} + \frac{\partial Q_y}{\partial y}$ at time t+1.

The scheme is thus practically completely centered except for the effect of the earth's rotation. The forcing functions which are input are indicated at $t-1$, but the system cannot distinguish the difference and assumed these at the level t , thus centered. The time step is limited by a stability condition

$$\frac{\Delta t}{\Delta s}\sqrt{gH_{max}} < 1/\sqrt{2} \qquad (6.69)$$

For small grid size and deep estuaries the time step becomes very small.

Leendertse (1967) used two approximations of Equations (6.52) through (6.54) which are used in succession. For the first set is used

$$u^{t+\Delta t} - u^{t} = -\Delta t\, F_1^{t+\Delta t} - \Delta t\, F_2^{t} \qquad (6.70)$$

$$v^{t+\Delta t} - v^{t} = -\Delta t\, G_1^{t+\Delta t} - \Delta t\, G_2^{t} \qquad (6.71)$$

$$\zeta^{t+\Delta t} - \zeta^{t} = -\Delta t\, H_1^{t+\Delta t} - \Delta t\, H_2^{t} \qquad (6.72)$$

where $F_1^{t+\Delta t} \doteq u\frac{\partial u}{\partial x} + g\frac{\partial \zeta}{\partial x}$ at time $t+\Delta t$ (part of the first, nonlinear term is taken at the lower level as sufficient data is not available other than through a predictor),

$F_2^{t} \doteq -fv + v\frac{\partial u}{\partial y} + R(x)$ at time t

$G_1^{t+\Delta t} \doteq fu + u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y} + R(y)$ at time $t+\Delta t$

$G_2^{t} \doteq g\frac{\partial \zeta}{\partial x}$ at time t

$H_1^{t+\Delta t} \doteq \frac{\partial (Hu)}{\partial x}$ at time t (part of this nonlinear term is taken at a lower time level as sufficient data is not available other than through a predictor),

$H_2^{t} \doteq \frac{\partial (Hv)}{\partial y}$ at time t

For the second set is used

$$u^{t+2\Delta t} - u^{t+\Delta t} = -\Delta t\, F_3^{t+2\Delta t} - \Delta t\, F_4^{t+\Delta t} \qquad (6.73)$$

$$v^{t+2\Delta t} - v^{t+\Delta t} = -\Delta t\, G_3^{t+2\Delta t} - \Delta t\, G_4^{t+\Delta t} \qquad (6.74)$$

$$\zeta^{t+2\Delta t} - \zeta^{t} = -\Delta t\, H_3^{t+2\Delta t} - \Delta t\, H_4^{t+\Delta t} \qquad (6.75)$$

where $F_3^{t+2\Delta t} \doteq -fv + u\frac{\partial u}{\partial x} + v\frac{\partial v}{\partial y} + R(x)$ at $t+2\Delta t$ (Parts of these nonlinear terms are taken at lower time levels)

$F_4^{t+\Delta t} \doteq g\frac{\partial \zeta}{\partial x}$ at $t+\Delta t$

$G_3^{t+2\Delta t} \doteq v\frac{\partial v}{\partial y} + g\frac{\partial \zeta}{\partial y}$ at $t+2\Delta t$ (Part of the nonlinear term taken at a lower time level)

$$G_4^{t+\Delta t} \doteq fu + u\frac{\partial v}{\partial x} + R(y) \text{ at } t+\Delta t$$

$$H_3^{t+2\Delta t} \doteq \frac{\partial(Hu)}{\partial x} \text{ at } t+2\Delta t \quad \text{(Part of the nonlinear term taken at a lower time level)}$$

$$H_4^{t+\Delta t} \doteq \frac{\partial(Hv)}{\partial y} \text{ at } t+\Delta t$$

This scheme is also nearly completely centered if multiples of $2\Delta t$ are considered. The exceptions are some of the nonlinear terms. The time step is not limited by a stability condition, but is limited by considerations of accuracy.

This multioperation method requires simultaneous solution of a system of equations. In each finite-difference equation (6.70) and (6.72), three unknown values of u and ζ exist, which are all situated on a row running from one side of the computational field to the other side. Consequently, systems of equations have to be solved, each system representing one row. Since each equation of such a system has only three unknown values, the system can rapidly be solved by recursion formulae, as is discussed by Leendertse (1967). Equation (6.71) can be solved explicitly for each point as all information is given. In the second operation, the Equations (6.74) and (6.75) are solved implicitly, but not in rows perpendicular to those of Equation (6.70) and (6.71). Consequently, the implicit solutions are always obtained in the direction of the velocity components which are to be solved in the stepping procedure.

In all two-dimensional computations, the description of boundary conditions is a considerable task, which becomes increasingly more difficult when the size of the computations increase. To reduce the programming effort of complicated fields, the FORTRAN program published by Leendertse (1967) determines the boundaries in the computation from a simple method of data insertion.

2.3.3 Numerical Simulation of Tidal Flow in Two Dimensions

At present the use of large two-dimensional tide models is still limited to direct computation. The available data are inserted in the program and a computation is made. The results, which are generally now in graphical form, represent flow and water level information for a limited period of time. The investigator will then compare observed data with the computed results and will find it necessary to adjust his input data, for example values of friction coefficients, in order to obtain better agreement. A next computation is made and the adjustment process is repeated. The rate at which a tide model can be adjusted to resemble the prototype depends on the extent of the field data, but a very important additional factor is the experience of the investigator and his access to the computer. An experienced investigator will make the adjustments far more rapidly than a novice in the field. A good understanding of the physics of the phenomena and an intimate knowledge of the behavior of the computational code with respect to physical phenomena are naturally requirements for any investigator using numerical models.

Models using several thousand computational points may require thirty to fifty adjustments, and the number of adjustments will increase with the number of grid points in the model. Thus, the access to the computer becomes critical for the progress of the investigation. Assuming that no code development is made, a rapid turn-around is essential. Unfortunately, the tide models with the associated advective-dispersion models have extensive computer memory requirements. The program queueing in computation centers generally discriminates against these large core-requiring computations, and results in an inefficient use of the investigator's time and of the time of his assistants. This is manifested, for example, in low ratios of computer cost to investigators' salaries.

Another serious impediment for the progress of the investigation is the handling of the numerical data, which have to be changed from experiment to experiment during adjustment of the model. With presently used models, which have arrays of only several thousand points, this is already a considerable task. The development of computers is still progressing at rates of an order of magnitude per five years for speed and memory size. Consequently, alternate ways of data handling have to be found. This data handling problem is a common occurrence in computation and has led to hardware and software developments which enable transfer of data from graphical form into digital form, and digital form into graphical form (Brown and Bush 1968, Davis and Ellis 1964). These developments make interactive simulation possible. However, considerable program development is still required. Such interactive simulation enables the investigator to follow the progress of the computation on cathode ray tubes on which computed data (e.g. tide levels and velocities) are presented simultaneously with measured data. The investigator can store the computation, change variables and continue, or backstep and restart from a previous time, and retain previous results on the scope together with results of the repeated computation and the measured data.

2.4 MASS TRANSPORT COMPUTATIONS

2.4.1 One-Dimensional Water Quality Computations

The balance equation for the mass concentration of a dilute substance moving in a channel of width b can be written

$$b\,\frac{\partial(Hc)}{\partial t} + \frac{\partial(Qc)}{\partial x} + b\,\frac{\partial\left(HD_x\,\frac{\partial c}{\partial x}\right)}{\partial x} + S = 0 \qquad (6.76)$$

where H = temporal depth, averaged over the cross section
Q = transport
c = mass concentration (mass per unit volume)
D_x = dispersion coefficient
S = the local source or sink of the mass per unit length

At present, this equation has not yet been solved numerically in the so-called conservation law form as discussed in Section 2.2.1. However, solutions in the nonconservative form have been obtained and are described in other chapters of this report (see, e.g. Chapter II, Section 3 and Chapter III).

In this discussion here, the Q will be assumed changing at a rather rapid rate by the tide. The finite-difference approximation which now will be used will be expressed upon a grid system that has the location of the Q situated between the grid point locations for the water levels ξ and the mass concentrations. The averaged depth up to the reference level of the water surface is taken at the same location as the Q , thus between the water level points ξ and the points of the mass concentration c . The latter are indicated with even values of m , and the depth and Q with odd values.

Consider a finite-difference equation at location m for the mass concentration

$$\begin{aligned}
&\frac{b}{\Delta t}\left[\left\{\left(h_{m-1}+h_{m+1}\right)/2+\xi_m^{t+1}\right\}c_m^{t+1}-\left\{\left(h_{m-1}+h_{m+1}\right)/2+\xi_m^{t}\right\}c_m^{t}\right]\\
&+\frac{1}{8\Delta x}\left[Q_{m+1}^{t+1}\left(c_{m+2}^{t+1}+c_m^{t+1}\right)+Q_{m+1}^{t}\left(c_{m+2}^{t}+c_m^{t}\right)-Q_{m-1}^{t+1}\left(c_m^{t+1}+c_{m-2}^{t+1}\right)\right.\\
&\left.-Q_{m-1}\left(c_m^{t}+c_{m-2}^{t}\right)\right]+\frac{b}{8(\Delta x)^2}\left[\left\{h_{m+1}+\frac{1}{2}\left(\xi_{m+2}^{t+1}+\xi_m^{t+1}\right)\right\}D_x\left(c_{m+2}^{t+1}-c_m^{t+1}\right)\right.\\
&+\left\{h_{m+1}+\frac{1}{2}\left(\xi_{m+2}^{t}+\xi_m^{t}\right)\right\}D_x\left(c_{m+2}^{t}-c_m^{t}\right)-\left\{h_{m-1}+\frac{1}{2}\left(\xi_m^{t+1}\right.\right.\\
&\left.\left.\left.+\xi_{m-2}^{t+1}\right)\right\}D_x\left(c_m^{t+1}-c_{m-2}^{t+1}\right)+\left\{h_{m-1}+\frac{1}{2}\left(\xi_m^{t}+\xi_{m-2}^{t}\right)\right\}D_x\left(c_m^{t}-c_{m-2}^{t}\right)\right]\\
&+S_m=0 \qquad (6.77)
\end{aligned}$$

It will be noted that in this equation for the location m , only three unknown values of the mass concentration appear, namely c_{m+2}^{t+1} , c_m^{t+1} , c_{m-2}^{t+1} . Consequently we have to solve a system of simultaneous equations, each with three unknown values of the concentration, except at the upper and lower ends where the equations include only two unknown values. The third which appears in the equation is a point in the boundary and should be given. A sweep method can solve such a system very rapidly.

As stated earlier, the computation of the tide has to be compatible with the expression for the conservation equation of the mass of the substance c . The required finite-difference expression for the equation of continuity can be obtained by introducing a unit value for all mass concentrations. This results in

$$\frac{b}{\Delta t}\left(\xi_m^{t+1}-\xi_m^{t}\right)+\frac{1}{4\Delta x}\left(Q_{m+1}^{t+1}+Q_{m+1}^{t}-Q_{m-1}^{t+1}-Q_{m-1}^{t}\right)=0 \qquad (6.78)$$

which is a central implicit expression that can be solved simultaneously with momentum equations. Both Equations (6.77) and (6.78) are conservative, and numerical integration in the spatial region will show no loss or gain in mass, except for the influxes at the boundaries, but these equations do not satisfy the conservation of quadratic properties. The dissipative and dispersive properties are already discussed in Section 2.2.3.

The concentrations generally are slowly varying in time, and the propagation speeds of the phenomena are much lower, an order of magnitude lower, than the propagation speed of the tidal wave. One would have the tendency to consider a computation with a much larger step for the water quality computation than for the tide computation, thus reducing the number of computations. It is difficult, if not impossible, to design the computations and have compatibility between the continuity equation of water and the mass balance equation of the substances in the water quality model, with different time steps in the models. In the first decennium of digital computation, restrictions in computer memory size and slow computation speeds forced investigators to use separation of tide and water quality computation, by storing the tide information on magnetic tape and subsequently solving the advective transport equations. At present, the computation of the tidal equations can be made in a shorter time than the transferal of data from magnetic tape, and this separation is no longer necessary.

2.4.2 Two-Dimensional Water Quality Computations

Two-dimensional computations can be made by use of the finite-difference approximation of the mass-balance equation derived in Chapter II

$$\frac{\partial(Hc)}{\partial t} + \frac{\partial(Huc)}{\partial x} + \frac{\partial(Hvc)}{\partial y} + \frac{\partial HD_x \frac{\partial c}{\partial x}}{\partial x} + \frac{\partial HD_y \frac{\partial c}{\partial y}}{\partial y} + S = 0 \tag{6.79}$$

The finite-difference equations used by Leendertse (1970) are two different sets which are solved simultaneously with the two sets of finite-difference equations of the tidal motion. After computation of the continuity equation, which is solved simultaneously with the momentum equation for the u velocity (6.70) and (6.72), the first mass balance equation is solved. The mass balance equation is computed using the same grid as the tide computation. Tide level ξ and the concentration c are situated on the same location, while the u velocity is situated between the water level grid points in the eastward direction and the v velocities are situated midway between the grid points in the northward direction. The water levels and concentration are at integer indices (m, n). The scheme uses water depth at locations in the center of four water level grid points, thus both indices indicating its location have integer and one-half values.

The first continuity equation used is

$$\begin{aligned}
&\left(\xi^{t+1}_{n,m} - \xi^{t}_{n,m}\right) \Delta t\Big[\left(\xi^{t}_{n,m-1} + \xi^{t}_{n,m} + h_{n-\frac{1}{2},m-\frac{1}{2}} + h_{n+\frac{1}{2},m+\frac{1}{2}}\right) u^{t+1}_{n,m-\frac{1}{2}} \\
&- \left(\xi^{t}_{n,m} + \xi^{t}_{n,m+1} + h_{n-\frac{1}{2},m+\frac{1}{2}} + h_{n+\frac{1}{2},m+\frac{1}{2}}\right) u^{t+1}_{n,m+\frac{1}{2}}\Big]/2\Delta x \\
&- \Big[\left(\xi^{t}_{n-1,m} + \xi^{t}_{n,m} + h_{n-\frac{1}{2},m-\frac{1}{2}} + h_{n-\frac{1}{2},m+\frac{1}{2}}\right) v^{t}_{n-\frac{1}{2},m} \\
&- \left(\xi^{t}_{n,m} + \xi^{t}_{n+1,m} + h_{n+\frac{1}{2},m-\frac{1}{2}} + h_{n+\frac{1}{2},m+\frac{1}{2}}\right) v^{t}_{n+\frac{1}{2},m}\Big]/2\Delta x \doteq 0
\end{aligned} \tag{6.80}$$

after which is solved the following equation:

$$\begin{aligned}
&\Big[c^{t+1}_{m} \left(h_{m-\frac{1}{2},n-\frac{1}{2}} + h_{m-\frac{1}{2},n+\frac{1}{2}} + h_{m+\frac{1}{2},n-\frac{1}{2}} + h_{m+\frac{1}{2},n+\frac{1}{2}} + 4\xi^{t+1}_{n,m}\right) \\
&- c^{t}_{m} \left(h_{m-\frac{1}{2},n-\frac{1}{2}} + h_{m-\frac{1}{2},n+\frac{1}{2}} + h_{m+\frac{1}{2},n-\frac{1}{2}} + h_{m+\frac{1}{2},n+\frac{1}{2}} + 4\xi^{t}_{n,m}\right)\Big]/4\Delta t \\
&- \Big[\left(\xi^{t}_{n,m-1} + \xi^{t}_{n,m} + h_{n-\frac{1}{2},m-\frac{1}{2}} + h_{n+\frac{1}{2},m+\frac{1}{2}}\right) u^{t+1}_{n,m-\frac{1}{2}} \left(c^{t+1}_{n,m-1} + c^{t+1}_{n,m}\right)
\end{aligned}$$

$$\begin{aligned}
&- \Big(\xi^t_{n,m} + \xi^t_{n,m+1} + h_{n-\frac12,m+\frac12} + h_{n+\frac12,m+\frac12}\Big)\, u^{t+1}_{n,m+\frac12} \Big(c^{t+1}_{n,m} + c^{t+1}_{n,m-1}\Big)\Big]/4\Delta x \\
&- \Big[\Big(\xi^t_{n-1,m} + \xi^t_{n,m} + h_{n-\frac12,m-\frac12} + h_{n-\frac12,m+\frac12}\Big)\, v^t_{n-\frac12,m} \Big(c^t_{n-1,m} + c^t_{n,m}\Big) \\
&- \Big(\xi^t_{n,m} + \xi^t_{n+1,m} + h_{n+\frac12,m-\frac12} + h_{n+\frac12,m+\frac12}\Big)\, v^t_{n+\frac12,m} \Big(c^t_{n+1,m} + c^t_{n,m}\Big)\Big]/4\Delta x \\
&- \Big[\Big(\xi^t_{n,m-1} + \xi^t_{n,m} + h_{n-\frac12,m-\frac12} + h_{n+\frac12,m+\frac12}\Big)\, D^{t+1}_{x_{n,m-\frac12}} \Big(c^{t+1}_{n,m} - c^{t+1}_{n,m-1}\Big) \\
&- \Big(\xi^t_{n,m} + \xi^t_{n,m+1} + h_{n-\frac12,m+\frac12} + h_{n+\frac12,m+\frac12}\Big)\, D^{t+1}_{x_{n,m+\frac12}} \Big(c^{t+1}_{n,m+1} - c^{t+1}_{n,m}\Big)\Big]/2\Delta x \\
&- \Big[\Big(\xi^t_{n-1,m} + \xi^t_{n,m} + h_{n-\frac12,m-\frac12} + h_{n-\frac12,m+\frac12}\Big)\, D^t_{y_{n-\frac12,m}} \Big(c^t_{n,m} - c^t_{n-1,m}\Big) \\
&- \Big(\xi^t_{n,m} + \xi^t_{n+1,m} + h_{n+\frac12,m-\frac12} + h_{n+\frac12,m+\frac12}\Big)\, D^t_{y_{n+\frac12,m}} \Big(c^t_{n+1,m} - c^t_{n,m}\Big)\Big]/2\Delta x + S_{n,m} = 0
\end{aligned} \tag{6.81}$$

In this equation only three unknown values of c occur, namely $c^{t+1}_{n,m+1}$, $c^{t+1}_{n,m}$, $c^{t+1}_{n,m-1}$. Thus Equation (6.81) can be written

$$A_m\, c^{t+1}_{n,m+1} + B_m\, c^{t+1}_{n,m} + C_m\, c^{t+1}_{n,m-1} = D_m \tag{6.82}$$

where A_m , B_m , C_m , and D_m can be derived from Equation (6.81). Thus for each row n , a system of equations of the type shown by Equation (6.82) exists, which can be solved directly by a sweep method.

For the second operation in the stepping order, Equation (6.75) is used for the equation of continuity. This formula is very similar to Equation (6.80), except that now the stepping goes from $t+1$ to $t+2$, and the terms with the V velocity are taken at the time level $t+2$, thus

$$\begin{aligned}
&\Big(\xi^{t+2}_{n,m} - \xi^{t+1}_{n,m}\Big)\,\Delta t - \Big[\Big(\xi^{t+1}_{n,m-1} + \xi^{t+1}_{n,m} + h_{n-\frac12,m-\frac12} + h_{n+\frac12,m+\frac12}\Big)\, u^{t+1}_{n,m-\frac12} \\
&\quad - \Big(\xi^{t+1}_{n,m} + \xi^{t+1}_{n,m+1} + h_{n-\frac12,m+\frac12} + h_{n+\frac12,m+\frac12}\Big)\, u^{t+1}_{n,m+\frac12}\Big]/2\Delta x \\
&\quad - \Big[\Big(\xi^{t+2}_{n-1,m} + \xi^{t+2}_{n,m} + h_{n-\frac12,m-\frac12} + h_{n-\frac12,m+\frac12}\Big)\, v^{t+2}_{n-\frac12,m} \\
&\quad - \Big(\xi^{t+2}_{n,m} + \xi^{t+2}_{n+1,m} + h_{n+\frac12,m-\frac12} + h_{n+\frac12,m+\frac12}\Big)\, v^{t+2}_{n+\frac12,m}\Big]/2\Delta x = 0
\end{aligned} \tag{6.83}$$

This equation is solved simultaneously with Equation (6.75). The second advective-diffusion equation is

$$
\begin{aligned}
&\Big[c_m^{t+2}\big(h_{m-\frac{1}{2},n-\frac{1}{2}} + h_{m-\frac{1}{2},n+\frac{1}{2}} + h_{m+\frac{1}{2},n-\frac{1}{2}} + h_{m+\frac{1}{2},n+\frac{1}{2}} + 4\xi_{n,m}^{t+2}\big)\\
&- c_m^{t+1}\big(h_{m-\frac{1}{2},n-\frac{1}{2}} + h_{m-\frac{1}{2},n+\frac{1}{2}} + h_{m+\frac{1}{2},n-\frac{1}{2}} + h_{m+\frac{1}{2},n+\frac{1}{2}} + 4\xi_{n,m}^{t+1}\big)\Big]/4\Delta t\\
&- \Big[\big(\xi_{n,m-1}^{t+1} + \xi_{n,m}^{t+1} + h_{n-\frac{1}{2},m-\frac{1}{2}} + h_{n+\frac{1}{2},m+\frac{1}{2}}\big)\, u_{n,m-\frac{1}{2}}^{t+1}\big(c_{n,m-1}^{t+1} + c_{n,m}^{t+1}\big)\\
&- \big(\xi_{n,m}^{t+1} + \xi_{n,m+1}^{t+1} + h_{n-\frac{1}{2},m+\frac{1}{2}} + h_{n+\frac{1}{2},m+\frac{1}{2}}\big)\, u_{n,m+\frac{1}{2}}^{t+1}\big(c_{n,m}^{t+1} + c_{n,m-1}^{t+1}\big)\Big]/4\Delta x\\
&- \Big[\big(\xi_{n-1,m}^{t+1} + \xi_{n,m}^{t+1} + h_{n-\frac{1}{2},m-\frac{1}{2}} + h_{n-\frac{1}{2},m+\frac{1}{2}}\big)\, v_{n-\frac{1}{2},m}^{t+2}\big(c_{n-1,m}^{t+2} + c_{n,m}^{t+2}\big)\\
&- \big(\xi_{n,m}^{t+1} + \xi_{n+1,m}^{t+1} + h_{n+\frac{1}{2},m-\frac{1}{2}} + h_{n+1,m+\frac{1}{2}}\big)\, v_{n+\frac{1}{2},m}^{t+2}\big(c_{n+1,m}^{t+2} + c_{n,m}^{t+2}\big)\Big]/4\Delta x\\
&- \Big[\big(\xi_{n,m-1}^{t+1} + \xi_{n,m}^{t+1} + h_{n-\frac{1}{2},m-\frac{1}{2}} + h_{n+\frac{1}{2},m+\frac{1}{2}}\big)\, D_{x_{n,m-\frac{1}{2}}}^{t+1}\big(c_{n,m}^{t+1} - c_{n,m-1}^{t+1}\big)\\
&- \big(\xi_{n,m}^{t+1} + \xi_{n,m+1}^{t} + h_{n-\frac{1}{2},m+\frac{1}{2}} + h_{n+\frac{1}{2},m+\frac{1}{2}}\big)\, D_{x_{n,m+\frac{1}{2}}}^{t+1}\big(c_{n,m+1}^{t+1} - c_{n,m}^{t+1}\big)\Big]/2\Delta x\\
&- \Big[\big(\xi_{n-1,m}^{t+1} + \xi_{n,m}^{t+1} + h_{n-\frac{1}{2},m-\frac{1}{2}} + h_{n-\frac{1}{2},m+\frac{1}{2}}\big)\, D_{y_{n-\frac{1}{2},m}}^{t+2}\big(c_{n,m}^{t+2} - c_{n-1,m}^{t+2}\big)\\
&- \big(\xi_{n,m}^{t+1} + \xi_{n+1,m}^{t+1} + h_{n+\frac{1}{2},m-\frac{1}{2}} + h_{n+\frac{1}{2},m+\frac{1}{2}}\big)\, D_{y_{n+\frac{1}{2},m}}^{t+2}\big(c_{n+1,m}^{t+2} - c_{n,m}^{t+2}\big)\Big]/2\Delta x + S_{n,m} = 0
\end{aligned}
\tag{6.84}
$$

Again a double sweep method is used to solve the system of simultaneous equations, of which each have three unknown values $c_{n+1,m}^{t+1}$, $c_{n,m}^{t+2}$, $c_{n-1,m}^{t+2}$.

The mass balance equation of the substance c is compatible with the continuity equation. Tests have shown that with a constant c, the error is of the ratio of 10^{-5} after a few thousand time steps using a field with several thousand points. The mass concentrations are conserved, but the water mass is not completely, due to a lower order approximation, as indicated in Section 2.3.2. Near sources, the equations are somewhat changed according to the principles presented in Section 2.2.5 to suppress the spatial oscillation which otherwise may occur at the upstream side of the source.

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DISCUSSION

HARDER: In my introduction to Section 1 of this Chapter I have tried to convey some of the conventional wisdom regarding digital computers, analog simulators, and analog computers. I have distinguished, for those who are not intimately familiar with them, between analog simulators and computers. Analog computers are going out of style, somewhat; they are certainly less popular now (1970) than they were before digital computers were important. But they have an advantage that digital computers have not quite yet attained in terms of the immediate interaction that's possible between the operator and the computer. I have indicated that as a considerable advantage, but one which is considerably offset by the disadvantage that analog computers generally can operate with only one dependent variable.

I'm sure that you will forgive me for not trying to indicate the solution techniques for each one of the equations of the other chapters. I've had to be content with giving an illustration of how one could apply analog simulators to a simple problem of tidal flow. In addition, I've given an indication of how one could apply analog computers (by which I mean a system in which we are trying to solve the equations explicitly), when one knows what the equations are, using integrators, adders, multipliers and other analog components. I have done that by making a brief application to the one-dimensional diffusion equation, by showing how one builds up the elements of such a system, after having broken the one-dimensional channel into segments. Then each segment can be simulated on the basis of the equation by, as I indicate, two sets of ganged potentiometers, two operational amplifiers, and one capacitor.

I made a few remarks on hybrid computation which won't be welcomed by the manufacturers of hybrid computing equipment. I think after some examination of the efforts that have been made that they have a principal advantage in saving intermediate results and recovering these results for subsequent insertion back onto the analog section. That is to say, you can save, through an analog-digital conversion, intermediate results in the digital form, and then reinsert them.

I then remarked on the economics of analog computation and pointed out that the generally available analog or hybrid-analog computing equipment is dreadfully expensive because of the exceedingly tight tolerances that are usually put on errors, typically one-hundredth of a percent. But it's not at all necessary or needed when the accuracy of our field measurements may be no better than 5 percent. Analog computing components are very cheap now, no more than $25 for integrators, maybe $35 for multipliers, if you're satisfied with a 1 percent accuracy.

THOMANN: Well, I'd just like to relate the worst experience I ever had in my life, trying to run diffusion-advection equations in coupled systems on three one-hundred-and-twenty amplifier, slaved analog computers. It was a horrible experience. We just couldn't get any kind of reproducibility, and I think you've talked about that in here. It was really hard to get that doggoned thing to work. Especially if the parameters are poorly behaved functions, and the function generators are the mechanical type that we have. Really quite an experience. It just didn't have the convenience of the digital computer.

I think the point that one can interact with the machine rapidly while he's doing verifications is not purely the domain of the analog. It may be that in the installation you have, you're in a situation with the digital computer that you have to wait a fair amount of time. That needn't be the case. You can interact.

HARDER: Well, I'm not suggesting that direct communication is the monopoly of hybrid or analog systems. This can be developed for digital systems. I think Jan knows of it. You can put the output on an oscilloscope directly from a digital computer.

PAULIK: Well, how about the use of time-sharing systems and the cathode ray display? Some of these are portable. They essentially use the telephone lines, to which you hook up an acoustical coupler and hook up a time-sharing terminal to a computer and display the results on a scope.

HARDER: I'm sure that these things are going to be even further developed in the future, and this is the reason I'm reluctant to recommend even considering analog computing equipment, but the advantage of analog computing equipment is that people who wish to work slowly can have the whole system spread out in front of them, and they are not chewing up valuable computer time as they are playing around with it.

I know that there are some things which you can do on digital computers which are not economical to do. The advantage of analog equipment is that the first cost is pretty nearly all of the cost. You can take your time about achieving verification, whereas, if you're paying so much an hour, you may not only get tired but also bankrupt by the time you finish your verification.

WASTLER: The models we have now are designed as digital models, basically. Would you care to comment on, for analog use, would there be merit in dropping all the way back to the basic equations and taking an entirely new tack which would be appropriate for an analog?

HARDER: Well, I can imagine that if you were doing analog computation, trying to carry forth seven dependent variables, that you'd have essentially seven parallel analog elements and these may be connected lengthwise to different reaches of the channel. Then there'd be cross connections between these seven variables in which each one of the variables would influence the rate reaction of each one of the others. Now this would be a tremendous amount of patching, but when you did it you would have a visual picture of exactly what you were doing. Now this you might not have so well if you'd had to write it out in FORTRAN. So there is certain visualization even in setting up the equations with analog type computers.

THOMANN: I think we should mention the use of some software that is around, provided by groups like IBM, like CSMP, Continuous System Modeling Program, where one essentially writes down the model in analog form but the entire program is executed digitally. In other words, you write down what Dr. Harder is talking about, but the program is implemented digitally. You don't have a real analog computer. You have a picture of what he's talking about. But the entire thing is carried out in a digital framework. In fact, in the early nonlinear nutrient-algal-zooplankton models that we looked at, we in fact modeled with CSMP, just to get the feeling of how the dynamics of the system behaved in simple spatially distributed models.

LEENDERTSE: The prime thing in this regard is that you can do all of these things on a digital computer. You can have all the interactions you want. You can have the graphical outputs immediately, if you have the proper equipment available. Even if you don't have, still there is the typewriter and printed output. You have to spend some time on writing the program for getting the output you want to have.

THOMANN: As far as the state-of-the-art is concerned, I don't really know anybody now that is using, in any sort of routine fashion, analog computation for water quality work.

BAUMGARTNER: Well, we have the experience that you've had with it.

WASTLER: We did a little bit on streams with the Streeter-Phelps analysis, but that was sort of a simple-minded approach to the thing.

THOMANN: I would say that the state-of-the-art now is that it has pretty well been discarded.

HARDER: It is possible, Bob, that the whole of the difficulty that you had was not with the computational scheme itself but with the problem. I mean not with the means of solving the problem but with the problem itself. You might have had the same problem with digital computers.

THOMANN: No, it was hardware problems.

* * *

LEENDERTSE: The subject of this second section is basically finite-difference schemes. It is evident that if you have a complex differential equation, you can have many, many approximations. The way to approach this is not by just starting to take finite differences, but to sit back and look very carefully and ask: what is the best way of approaching, and the best way of finding the approximations? Now we have, unfortunately I would say, the formulation of the problem in partial differential equations and the formulation of the difference equations going hand-in-hand. It is quite noticeable from the work that has been done up to now in formulating these, and you find it in the previous sections also, that it has been cued quite a bit to the analytical thinking that people have. I should say we have to be careful that we don't go along those lines, in order to avoid quite serious shortcomings in our solutions.

In setting up our computational schemes we have to satisfy the same things, or we try to satisfy the same things, as when we set up our partial differential equations. We have conservation of mass, conservation of momentum, and conservation of constituents. I gave an example here of how you look at conservation of mass; how you integrate over time and space in the partial differential equation, and how you do that in the finite-difference approximation. By the way, every scheme which we are working with right now actually doesn't conserve mass. Only but very few schemes really do that.

Another problem is the stability of computation. You will find in the literature that people are generally quite concerned about it. This is not necessary. If you really make an analysis of the problem, in the way I said at first here, you will find that you can immediately design a scheme which is stable. There's one exception, and that is the problem of the nonlinear terms, for example, advection terms. They very often generate instability just by the fact that you get product terms of very short periodic fluctuation, which then start to be amplified.

CALLAWAY: Do you get that in the small scale grid that you are using, too?

LEENDERTSE: No, due to the fact that I use filtering techniques. I have explained here how those terms come into existence, and the way you can get rid of them is actually by taking one of the nonlinear terms in a manner that you filter out the very short wavelengths throughout.

Some other problems incurred in computations are the dissipative and dispersive effects. Now "dispersive" in this particular subject maybe is not a very good name for it because you might confuse this with dispersion, but this is the way the term has been used in mathematics. That a system is dispersive means that the velocity of propagation of the phenomena becomes dependent upon the mode of computation. The dissipative effect is like when a certain periodic phenomenon, which is not itself dissipated, becomes dissipated by the scheme, in other words, you get a kind of numerical dissipation. It is generally possible to have no dissipative effect in your computations. I think that's the right way to look at our problems. However, you cannot get rid of the dispersive effects. So certain phenomena will not propagate properly in our computations. I have given some of the analysis here and presented some of the ideas on how you handle that, and how you can compute how much this dispersion is. In other words, you set up a scheme, a finite-difference approximation, and in addition you look at the grid sizes. From that and from the information provided here you can get a pretty good idea what the computational solutions will look like and how they will behave.

Discontinuities are another problem we have. Those occur, of course, at the points of injection, and there is really not a very good way of handling these. All our computational methods, all our finite-difference methods, are based upon fairly slowly varying phenomena. This is also slowly varying in the spatial sense. If you have a discontinuity at a discharge, you get computational effects in the results. You have to be aware of this.

Then in Section 2.2.6, I have some comments on higher order schemes. All the modeling which has been done, as far as I can see, has been approached in the way ordinary differential equations are approached. However, we have partial differential equations, and as a consequence we do not have to worry too much about the accuracy of the say, time-varying concentrations in relation to the accuracy of the other terms. Section 2.2.7 treats the use of conservation laws to obtain nonlinear stability. I indicated earlier that linear stability you can handle rather rapidly, and nonlinear stability you can do something about, but there is now a rather clean-cut way, by imposing another condition upon your finite-difference scheme, to assure yourself that you get no nonlinear instabilities. As far as I know this has not been applied yet anywhere except in computations of the advection terms in momentum equations.

Now in 2.3.1, I really didn't give a detailed example of that for the following reason. I went through the literature, and there is not really one scheme which conserves mass in one-dimensional computations. I feel this is rather a shortcoming in our present state-of-the-art. We should have a very good model of one-dimensional computations which is conservative.

In two-dimensional computations, there are several schemes available. We do not have as many problems with two-dimensional computations as with one-dimensional computations. In this sense the one-dimensional computation is more difficult than the two-dimensional computation. I explain how to get to your method, something along my own method. I may point out, however, that in order to conserve energy, for instance, or momentum, you do have to write the equation in the form of (6.55). We obtain the two-dimensional computation in very much the same way. We have very much the same problems as with adjustment in tidal models. It is a very time consuming task to look at all the outputs that you have and to decide where to put a little more resistance in or where to put a little more depth in.

Then Section 2.4 discusses mass transport. I have given here a scheme (I think it is also rather new) which conserves the mass as far as I can see. It does not conserve the quadratic terms, the mean variance of concentrations, very well. Then the discussion goes into the two-dimensional water quality computations and describes the formulas which I have been using.

WARD: For the record, could you discuss your comment that the use of box or cell models is not advisable.

LEENDERTSE: The use of such methods fixes immediately the finite-difference equations without regard to computational effects. I think that is just to write the answer for it. So you force upon yourself a solution technique with all the possible shortcomings you have. That is not the way to handle it. You should first look at the partial differential equation, or maybe an integro-differential equation if you want to be more sophisticated, and then go from there and design your scheme. If you design your scheme immediately, you make take lower order approximations, force upon it lower approximations, which aren't necessary.

BAUMGARTNER: Earlier in the day when we were talking about some bays or harbors where things might be well-mixed. I thought there was some indication that this might be a case where we use something that would turn out to be a box model. I don't know if I recall your shaking your head or which way it was going, but I felt otherwise that we had a pretty general consensus that this might be an acceptable way to handle it.

LEENDERTSE: In that case, it may be so that you can use it, that you can make a box model, but it just happens to be so. You just came out all right. Maybe the advective transport and the diffusion was not really important. But that is not the way you should approach it. You should approach it from the partial differential equations, and then have a careful look at what are the various contributions.

WARD: I think that's very important.

RATTRAY: Don't compromise with reality before you have to.

WARD: Right. Stick with the differential equation.

RATTRAY: And even in that case of having a well-mixed bay, it seems to me that you have one problem in matching the boundary conditions. The fluxes of water and the other concentrations aren't too realistic. Even though the box itself might well represent a well-mixed bay, representing the exchanges as pipelines might not be so good.

PRITCHARD: I'd just like to argue this case a little, from the standpoint that when you make a finite-difference statement of a differential equation, you are, in fact, building a box model. And so what we are talking about is the size of the grid, for instance in the

Thomann model. There is considerable discussion in Orlob's papers about the problems of how you take the finite differences, because you are dealing with real steps and these are not real linear gradients. This is where you get in trouble with the box model. It is the problem of having to have assigned values to the boundaries, or in terms of how you evaluate the parameters in the boxes, and how you take the differential.

LEENDERTSE: In this particular case, the scheme that is basically used there is likely unstable, just by this assumption that is being made. If you have a four part stepping scheme, so you go from one time level and you compute, from the information which is available, forward eight times, that scheme is basically unstable, always unstable. You can make it stable by doing something to the gradients, that's described in Section 2.2.2 or 2.2.3, so then you start matching and you do something that is really not correct. If you want to really build a scheme you go from the partial differential equations, and you are not concerned with the box concept at first.

PRITCHARD: When you set up the grid of known information, you are taking finite steps. Now, you introduce errors with that grid if the parameters really are not linearly varying in space, and you estimate the differential by delta-over-delta approximately.

LEENDERTSE: But it is not the only way. You see, you have many possibilities as to how you can take the differences. So you want to design your scheme in such a manner that you get the right characteristics of the computation or the most preferred. Of course, you want to have stability in the computation, but you don't want to take a scheme which is so stable that it diffuses everything.

PRITCHARD: I think I am following that. But what I am really perhaps saying is that I think there has been a number of so-called computer mathematical models which in effect are box models in that the time steps and space steps are sufficiently large so that there is a real question of how you take the difference.

What I am concerned with is the scale of the input information. Just from the standpoint of the amount of data that we can get, we're limited in space in what kind of differences we can formulate, so that I think we are down to having to make some approximations which essentially become almost box-like models. This is my point. Not that one wants to do this if you could solve the things, but I am saying in the meantime, until we can, I think we are faced with having to make our best estimates at the present time on the models that we have.

LEENDERTSE: Yes. Still I would first look at it from the other way. Go from the partial differential equations and do it in that manner, and then prefer to make your choice not in terms of, let's say, $u\,\partial u/\partial x$ or something like that, in those terms, but combine these as cross-product terms. The cross-product terms in the computations do handle much better while many of the other terms don't.

RATTRAY: Well, Don, I think you said the same thing in a different way earlier. What you want to do if you have such a situation is to try to integrate the differential equations over some region of the section or volume.

PRITCHARD: Right. That's exactly what I would do. Absolutely.

RATTRAY: And you have an explicit expression for the boundary exchanges, instead of estimating it some other way. That's different from a box-model.

PRITCHARD: Well, all right. But you still come out with dividing the system up into a finite number of steps. That's my point.

LEENDERTSE: But what you can do is, if you would look at the box-model, you can take the integral equations and integrate over the boxes and maybe do some corrections on that.

PRITCHARD: That is what I am doing. Starting with the differential equations and integrating over finite segments.

LEENDERTSE: Yes. Well, that's justified.

HARDER: In defense of Jan's criticism of the box approach, I think you might find if you used a simple-minded box approach that you wouldn't by that means itself be able to distinguish the advantages and disadvantages of implicit, explicit and mixed-mode types of computation.

PRITCHARD: Yes. When you do have a system of equations, there are advantages to implicit solutions.

HARDER: That you would not see from a box approach.

LEENDERTSE: With reference to implicit or explicit scheme, I am very much convinced that the multioperational approaches are the way that we have to go. Also, in the three-dimensional case. The multioperational method, where you have more than one approximation to the partial differential equations, gives much more flexibility in the mode of computation. If you have an implicit scheme, it is very often difficult to solve. If you take a multioperational approach for which you have more than one approximation for the partial differential equations, you have a certain amount of choice for, let's say, making it implicit in one direction, and in the next operation you take it implicitly in the other direction. The mathematical way of handling it is available.

HARDER: As an example, let me point out that, if you have a dynamic equation and a continuity equation which have to be satisfied at all times, you can use an explicit scheme for the dynamic equation and then turn around and use an implicit scheme for the continuity equation, and then step alternately in this direction. It helps very often in accuracy and stability. But it has to be done with a good deal of sophistication, as Jan has applied to it.

CHAPTER VII

CASE STUDIES

George H. Ward, Jr.
and
William H. Espey, Jr.

1. INTRODUCTION

While the emphasis of the preceding chapters has been on the principles of estuarine water quality modeling, the concern of this chapter is with the practice of modeling as exemplified by specific estuarine modeling projects. This chapter consists therefore of a collection of surveys, with the stress upon implementation of models and their adequacy in predicting water quality. The attempt is made to present accounts of these projects without injecting any judgments on the work, so that each case study is, in effect, a summary of the available documentation on that project. The selection was made so as to encompass a variety of modeling techniques as well as to represent different types of estuaries. The choice was limited largely to major estuarine systems or major modeling projects where, in general, sufficient resources were available to exploit the capabilities of the models.

As this chapter is concerned principally with those applications offering insight into the present ability of models to reproduce nature, a number of topics are not discussed in detail, such as the employment of modeling for management decisions, e.g. least cost optimization, allocation of waste loading, alternative treatment levels, or the delineation of quality standards. Two applications of current interest, viz. modeling of the effects of streamflow regulation and of the effects of physiographic modification, have been given particular prominence. Existing capabilities for modeling these effects are, of course, limited by the adequacy of present models as delineated in the preceding chapters, especially with regard to hydrodynamic phenomena. However, the examples in this chapter serve to illustrate the extent and success with which existing techniques have been applied to these problems, as well as to others. Ultimately, it is in the applications that the practical capabilities and the practical limitations of present estuarine modeling are demonstrated.

2. THE THAMES

The study of pollution in the Thames Estuary, which was undertaken by the Thames Survey Committee through the Water Pollution Research Laboratory and which culminated with the Water Pollution Research Laboratory (1964) report, had the objective of developing predictive mathematical models upon which the future management of the estuary could be based. The study received its principal impetus from public complaints about the production of malodorous gases, principally hydrogen sulfide, arising from anaerobic reaches of the Thames. The basic problem in the estuary was the concentration of dissolved oxygen, and therefore DO was the parameter of principal interest in the study.

2.1 PHYSIOGRAPHY AND HYDROGRAPHY

The physical characteristics of the Thames are summarized in this section. The reader is referred to WPRL (1964) for details. The estuary proper from the mouth to Teddington Weir, the limit of tidal influence, is depicted in Figure 7.1. The variation of depth and cross-sectional area is shown in Figure 7.2. A typical tidal range below London Bridge is 15 feet, decaying rapidly to zero above the bridge (Figure 7.3).

The principal source of inflow is the river Thames, and this flow is gauged at Teddington Weir (which is below the major municipal withdrawals) to be nominally 1,000 MGD. Seasonal trends in the gauged inflow are displayed in Figure 7.4, which shows the monthly inflows averaged over many years of record. The daily records for a given year of course exhibit considerably more irregularity. Additional freshwater inflows below Teddington Weir are contributed by the tributaries, storm sewers, and municipal and industrial effluents. Figure 7.5 shows the total net seaward flow below Teddington Weir for four distinct inflow conditions. The curves are numbered with the ordinate value 20 miles above the Bridge, viz. the gauged flow at Teddington Weir. Combining these results with the cross-sectional areas of Figure 7.2, one can estimate the net velocity due to inflow (Figure 7.6).

The Thames is vertically well-mixed and is typically only slightly stratified. The vertical distribution of salinity at high water (spring tide) is given in Figure 7.7 with the equivalent distribution for the Tees (see also Stommel and Farmer 1952, Section 7.21). The degree of vertical salinity stratification is further indicated in Table 7.1. Some typical longitudinal distributions of salinity are shown in Figure 7.8.

2.2 POLLUTING LOADS

The predominate source of pollution in the Thames is municipal effluents and most of the significant loads are discharged below Teddington Weir. The distribution of BOD loads for two different sampling periods according to the nature of the source are given in Table 7.2. It is evident that municipal sewage contributes nearly 80% of the total BOD load, the remainder being divided nearly equally between industrial discharges and freshwater inflows. Typical (five-day) BOD distributions are shown in Figure 7.9, and in Figure 7.10 are displayed some typical longitudinal distributions of DO, nitrogen compounds and salinity. The flow at

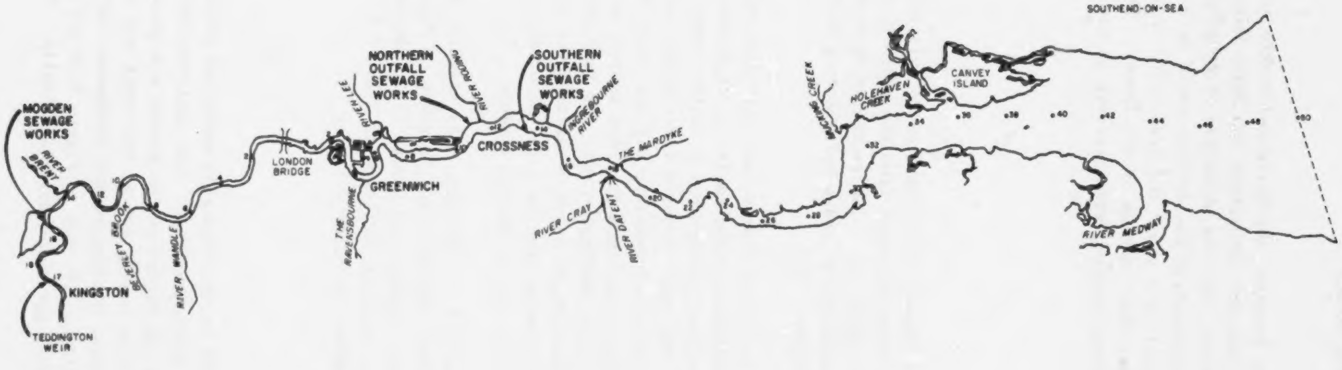
MOGDEN SEWAGE WORKS
RIVER BRENT
TEDDINGTON WEIR
KINGSTON
BEVERLEY BROOK
RIVER WANDLE
LONDON BRIDGE
THE RAVENSBOURNE
RIVER LEE
GREENWICH
NORTHERN OUTFALL SEWAGE WORKS
RIVER RODING
CROSSNESS
SOUTHERN OUTFALL SEWAGE WORKS
INGREBOURNE RIVER
THE MARDYKE
RIVER CRAY
RIVER DARENT
MUCKING CREEK
HOLEHAVEN CREEK
CANVEY ISLAND
SOUTHEND-ON-SEA
RIVER MEDWAY
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Fig. 7.1 Thames Estuary. Numbers on Axis are Distances (s.m.) from London Bridge. After WPRL (1964).

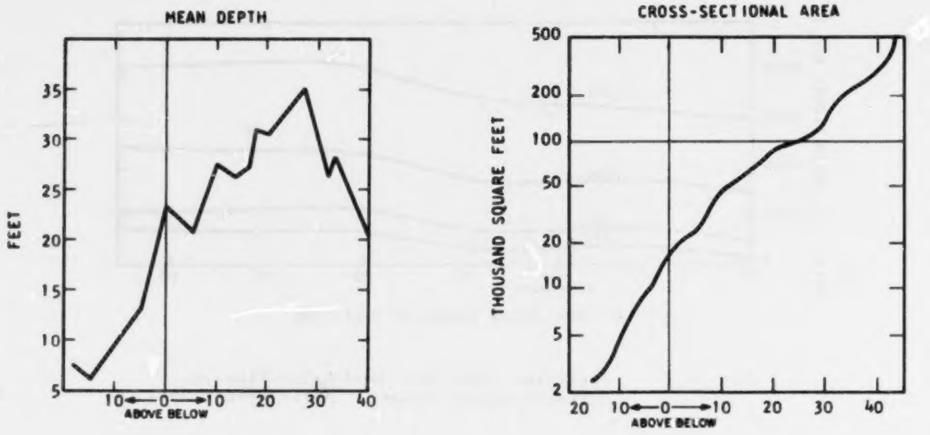


Fig. 7.2 Physical characteristics of Thames as a function of distance (s.m.) from London Bridge. After WPRL (1964).

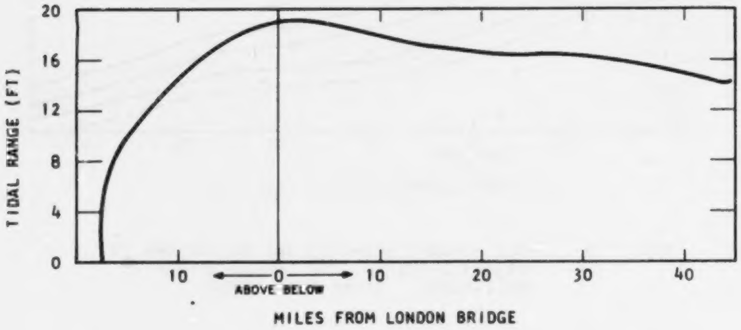


Fig. 7.3 Range of water level during average tidal cycle in absence of surface disturbance. After WPRL (1964).

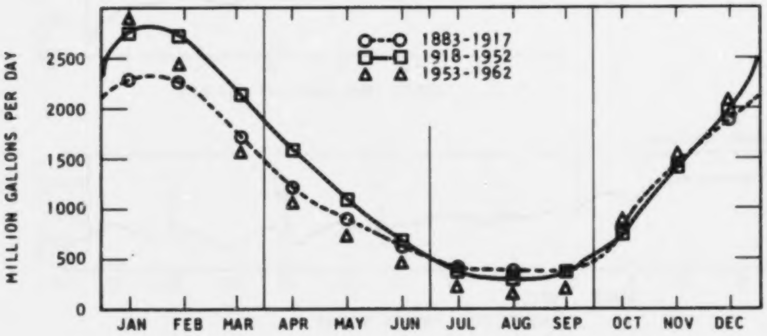


Fig. 7.4 Monthly average values (over indicated period) of gauged flow at Teddington. After WPRL (1964).

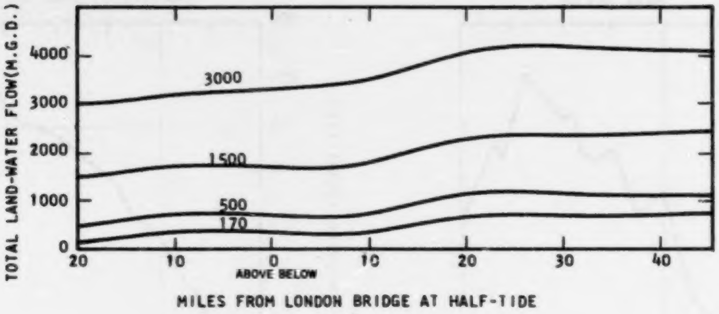


Fig. 7.5 Estimated total net land-water flow vs. distance along estuary. After WPRL (1964).

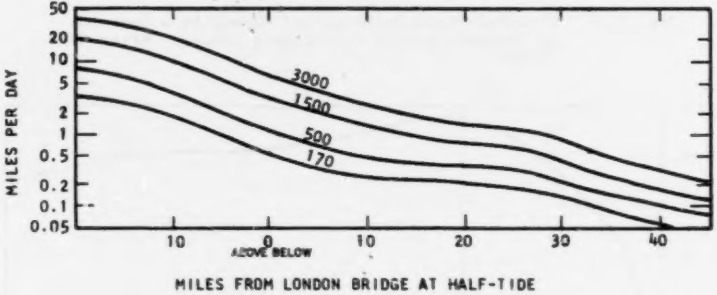


Fig. 7.6 Net seaward velocity due to inflows of Figure 5 (miles from London Bridge at half-tide). After WPRL (1964).

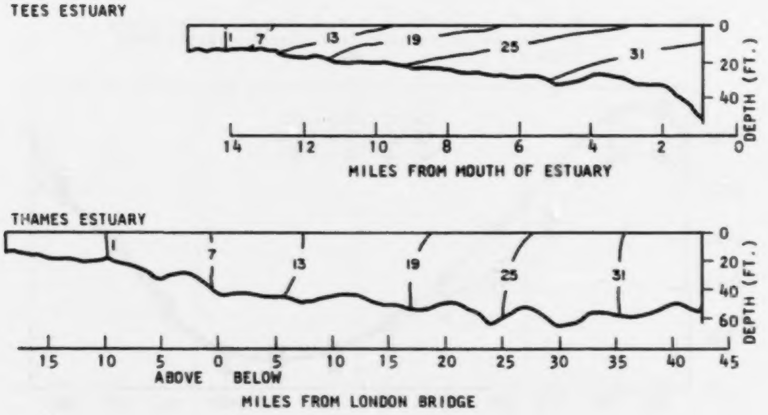


Fig. 7.7 Isohaline contours (o/oo) at high water of a spring tide in the Tees and Thames Estuaries. After WPRL (1964).

TABLE 7.1

DISTRIBUTION OF SALINITY (o/oo) IN THAMES ESTUARY

From WPRL (1964)

POSITION (Miles Below London Bridge)	DEPTH (ft)	SURFACE SALINITY	SALINITY NEAR MID-DEPTH		SALINITY NEAR BOTTOM		SALINITY DIFFERENCE BETWEEN NEAR-BOTTOM AND SURFACE
			Depth	Salinity	Depth	Salinity	
Low water, neap tides, 6-7 April 1949							
0.4	27	0.18	15	0.18	26	0.18	0.00
3.1	27	0.55	15	0.46	26	0.64	0.09
4.9	26	0.92	15	1.19	25	1.19	0.27
7.0	27	1.73	15	1.93	26	2.38	0.65
9.3	28	3.91	15	3.91	27	4.00	0.09
11.7	29	5.54	15	6.26	28	6.44	0.90
13.8	38	7.88	15	8.24	30	7.97	0.09
16.5	38	9.69	15	9.69	30	10.41	0.72
18.7	41	11.40	15	11.40	30	12.30	0.90
21.6	39	13.57	15	13.75	30	14.47	0.90
23.9	43	15.19	15	15.37	30	15.55	0.36
26.2	39	16.46	15	16.64	30	16.82	0.36
27.7	38	17.36	15	17.90	30	18.53	1.17
29.4	49	18.44	15	18.35	30	19.07	0.63
31.1	39	19.70	15	20.07	30	21.33	1.63
33.2	--	22.05	15	22.68	30	23.95	1.90
36.0	34	23.77	15	24.13	30	25.12	1.35
38.7	38	26.02	15	26.56	30	26.65	0.63
40.9	37	27.20	15	27.20	30	27.38	0.18
43.1	42	28.55	15	28.64	30	29.36	0.81
High water, spring tide, 27 April 1949							
26.2	53	23.86	25	23.40	50	24.94	1.08
28.4	52	26.02	25	26.92	50	26.74	0.72
30.5	52	27.11	25	28.01	50	28.55	1.44
33.2	53	29.27	25	29.27	50	29.27	0.00
36.0	53	30.17	25	30.53	50	30.90	0.73
38.7	51	30.99	25	31.26	50	31.26	0.27
40.9	51	31.44	25	31.44	50	31.26	-0.18
43.1	51	32.25	25	32.34	50	32.52	0.27

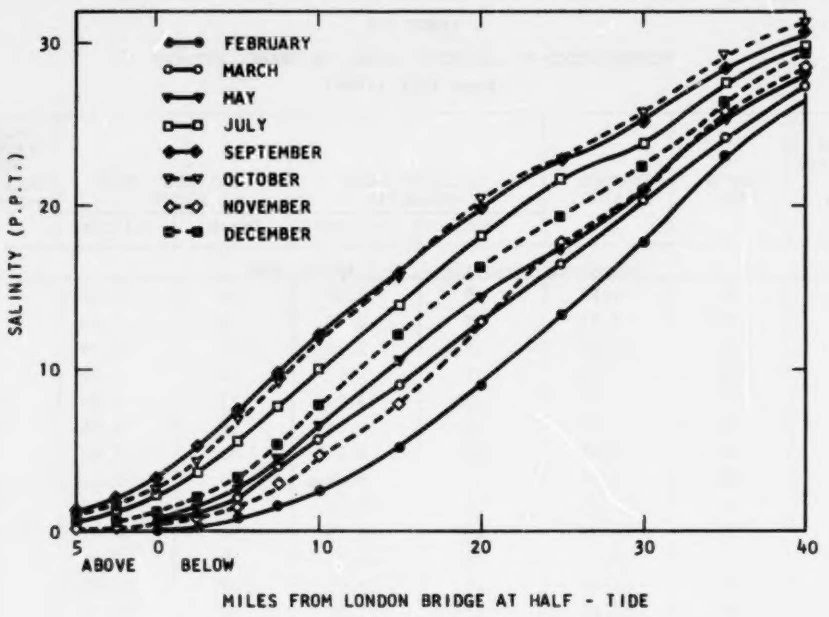


Fig. 7.8 Average salinity distribution along Thames for selected months in 1953. After WPRL (1964).

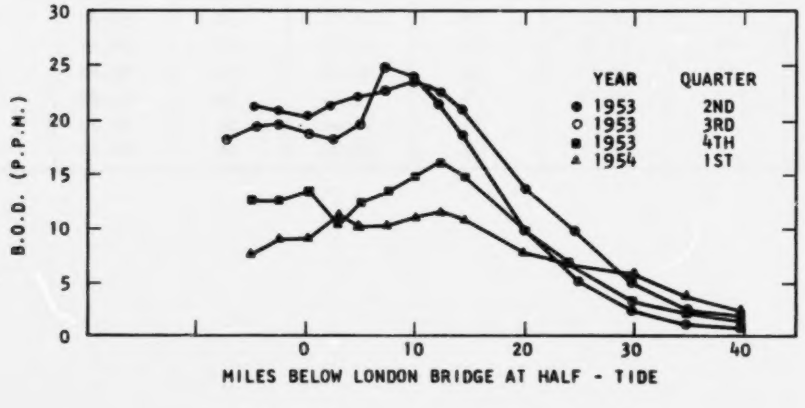


Fig. 7.9 Quarterly average distributions of B. O. D., April 1953 to March 1954. After WPRL (1964).

FIGURES IN PARENTHESES ARE PERCENTAGES OF TOTAL

	1950-53	1960-62
SEWAGE EFFLUENTS	331 (79)	270 (78)
STORM SEWAGE	8.5 (2)	11 (3)
DIRECT INDUSTRIAL DISCHARGES	52 (12)	31† (9)
FRESH-WATER DISCHARGES	28* (7)	36 (10)
TOTAL	420 (100)	348 (100)

*DATA MAINLY FOR 1952-53. †DATA FOR 1962.

Table 7.2 Estimated average B. O. D. loads (tons/day) discharged to estuary from Teddington to 32 miles below London Bridge during two periods. From WPRL (1964).

Teddington on 31 August 1954 (Figure 7.10a) was representative of summer conditions, ca. 400 MGD, while that on 23 February 1954 (Figure 7.10b) was ca. 2500 MGD, representative of wet winter conditions. The variation of these parameters through the anaerobic reach should be especially noted. The increase in inorganic nitrogen 10 miles below the Bridge is due to effluent discharges in this area. The decay of nitric nitrogen (nitrate) indicates that it is reduced in the anaerobic area, and the decrease in ammoniacal nitrogen establishes that free nitrogen rather than ammonia is the reduction product.

The Thames is also subject to large discharges of heated effluents, averaging 3×10^{11} BTU/day of which 75% is due to cooling water from power stations, the remainder being the combined effects of freshwater discharges, municipal and industrial effluents, and biochemical activity. Some typical longitudinal distributions of temperature are given in Figure 7.11.

2.3 MODELING TECHNIQUES

The approach to the mathematical modeling of quality parameters which was employed in the Thames study possesses some features that differ from the approaches discussed in preceding chapters and thereby deserves a relatively detailed description. The incorporation of the effects of tidal mixing is particularly noteworthy in that the advective-diffusion equation was abandoned in favor of a probabilistic approach.

After one tidal cycle, the water originally within a small interval $\delta \ell$ of a point 0 (measured on the longitudinal axis) is represented as being spread either side of 0 according to a distribution curve associated with the point 0. Each point on the estuary axis is thought of as possessing such a distribution curve which completely characterizes the mixing at that point. The particular form assumed for the distribution is not important so long as its first and second moments agree with the "real" distribution, because after several successive tidal cycles approximately the same dispersion pattern results. This is demonstrated graphically by Figure 7.12. For this reason a rather simple form of the distribution is assumed, viz. that after a given number (one, say) of tidal cycles, a fraction P_1 of the water originally at 0

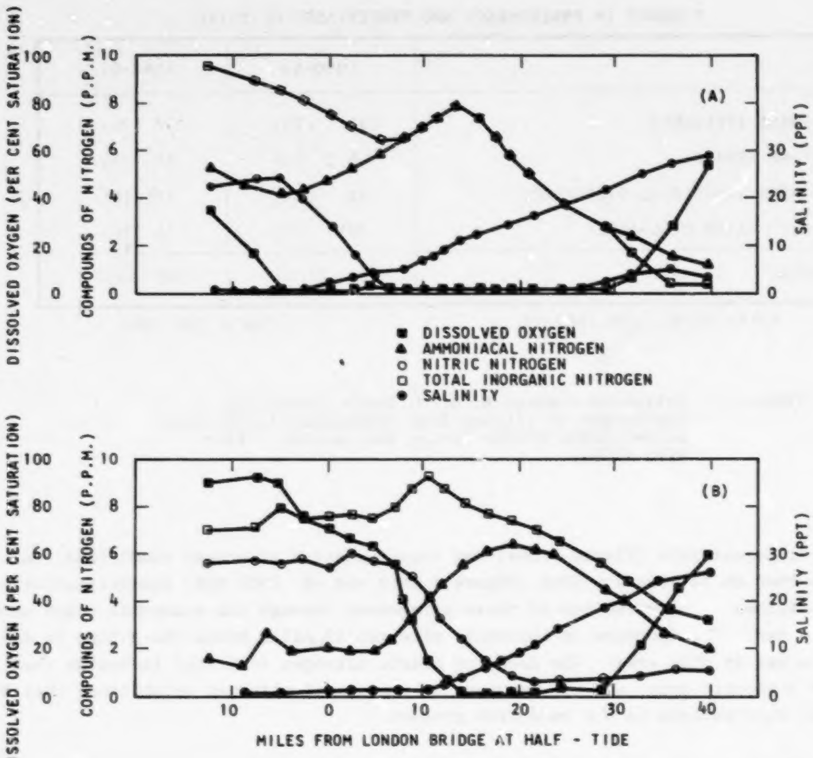


Fig. 7.10 Distribution of dissolved oxygen, inorganic nitrogen compounds, and salinity in Thames on (a) 31st August and (b) 23rd February 1954. After WPRL (1964).

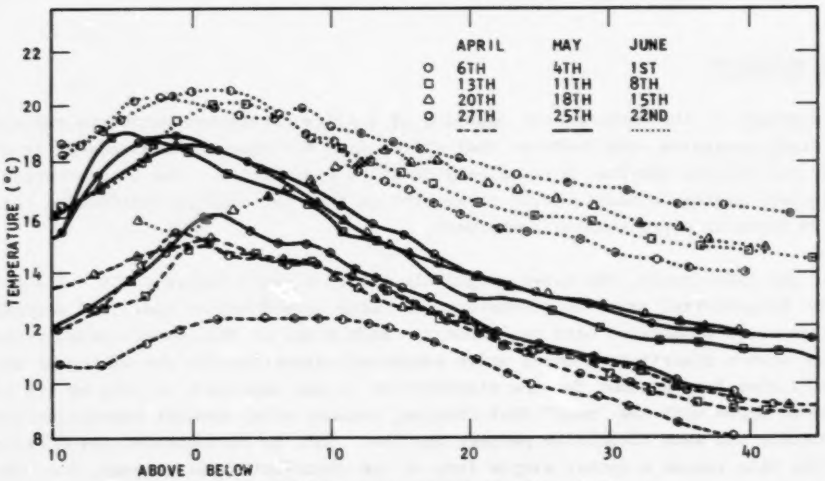


Fig. 7.11 Results of weekly measurements of temperature in Thames Estuary, April-June 1954. After WPRL (1964).

is spread uniformly over a distance L downstream from 0, P_2 is spread uniformly L upstream from 0, and $1 - P_1 - P_2$ remains within the original interval $\delta\ell$ of 0 (see Figure 7.13). The distance L is called the "mixing length" (but bears no relation to Prandtl's theory). The value of L is not thought to be especially crucial and is therefore taken to be an integral number of miles "rather less than the average tidal excursion" and is assumed invariant along the estuary. Characterization of the mixing now reduces to the problem of finding P_1 and P_2 as a function of longitudinal distance along the estuary. A degree of judgment is required in that if $P_1 + P_2$ is found to exceed unity then L must be increased, and if $P_1 + P_2$ is "excessively small" L must be decreased.

Computation of the mixing constants P_1 and P_2 is accomplished by the use of two conservation principles:

(i) The flux of salt upstream across any cross section in a given time period is equal to the total salt above the cross section at the end of the time period less the amount of salt present initially (neglecting saline discharges, as was found permissible for the Thames).

(ii) Mixing alone does not effect a net transfer of water across any cross section.

During one tidal cycle the salt carried upstream past a point x is

$$\int_0^L \bar{S}\,(x+\ell)\ A(x+\ell)\ P_2(x+\ell)\ \frac{L-\ell}{L}\ d\ell$$

where $\bar{S}$ is the average salinity over the tidal cycle. Similarly the total salt carried downstream past x is (since $\ell < 0$)

$$\int_{-L}^{0} \bar{S}\,(x+\ell)\ A(x+\ell)\ P_1(x+\ell)\ \frac{L+\ell}{L}\ d\ell$$

The net accumulation of salt ΔW above x in one tidal cycle is therefore

$$\Delta W = \frac{1}{L}\left\{\int_0^L \bar{S}(x+\ell)\ A(x+\ell)\ P_2(x+\ell)\ [L-\ell]\ d\ell - \int_{-L}^{0} \bar{S}(x+\ell)\ A(x+\ell)\ P_1(x+\ell)\ [L+\ell]\ d\ell\right\} - \overline{Q(x)\ S(x)}$$

where Q(x) is the net discharge above x in one tidal cycle and the overbar denotes the mean value over the tidal cycle. It was found (WPRL 1964, p. 401) that ΔW could be neglected. Using this fact and writing $X = AP_1$ and $Y = AP_2$ for convenience, the first conservation principle becomes

$$\frac{1}{L}\left\{\int_0^L \bar{S}(x+\ell)\ Y(x+\ell)\ [L-\ell]\ d\ell - \int_{-L}^{0} \bar{S}(x+\ell)\ X(x+\ell)\ [L+\ell]\ d\ell\right\} - \overline{Q(x)\ S(x)} = 0 \qquad (7.1)$$

The second conservation principle, by the same reasoning, is stated

$$\int_0^L Y(x+\ell)\ [L-\ell]\ d\ell - \int_{-L}^{0} X(x+\ell)\ [L+\ell]\ d\ell = 0 \qquad (7.2)$$

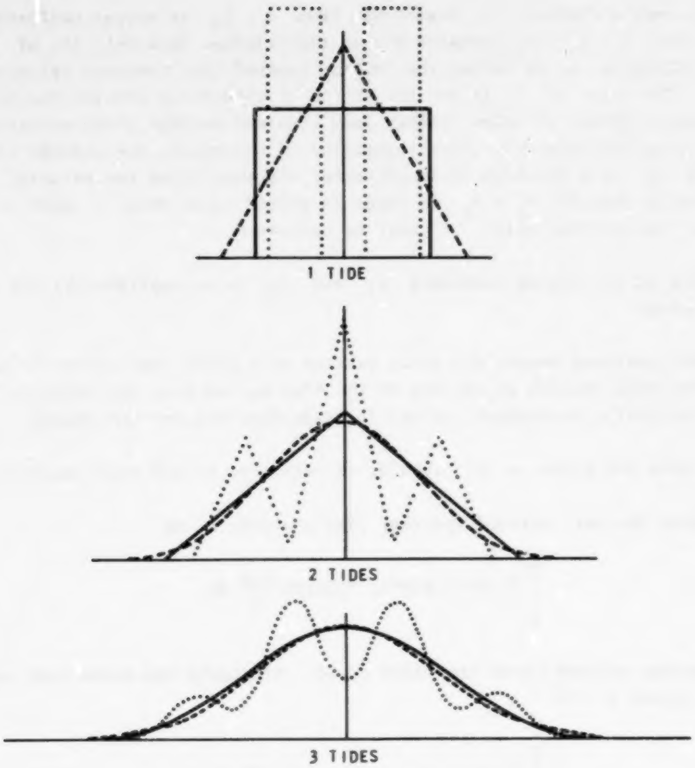


Fig. 7.12 Distribution of water after 1, 2, and 3 tides using three representations of symmetric mixing, each with same second moment. After WPRL (1964).

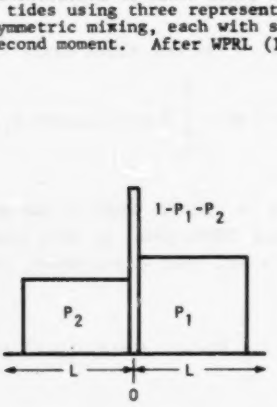


Fig. 7.13 Representation of distribution after one tidal cycle of unit mass of water originally at 0, neglecting net displacement due to freshwater inflow. After WPRL (1964).

Calculation of X and Y is equivalent to calculation of the mixing parameters P_1 and P_2. X and Y were calculated for the Thames using measured average salinities and discharges together with numerical integration of (7.1) and (7.2) for one-mile increments along the estuary. L was taken to be 6 miles (for a mixing period of one tidal cycle), and the mixing parameters were computed to be as displayed in Figure 7.14.

Once P_1 and P_2 as functions of x have been determined, the salinity distribution can be calculated from Equation (7.1) for a given inflow conditions; P_1 and P_2 are also used to compute the effect of tidal mixing on other parameters as described below. Representation of the mixing by this method was applied to average tides, so that the difference between, say, spring and neap was effectively neglected.

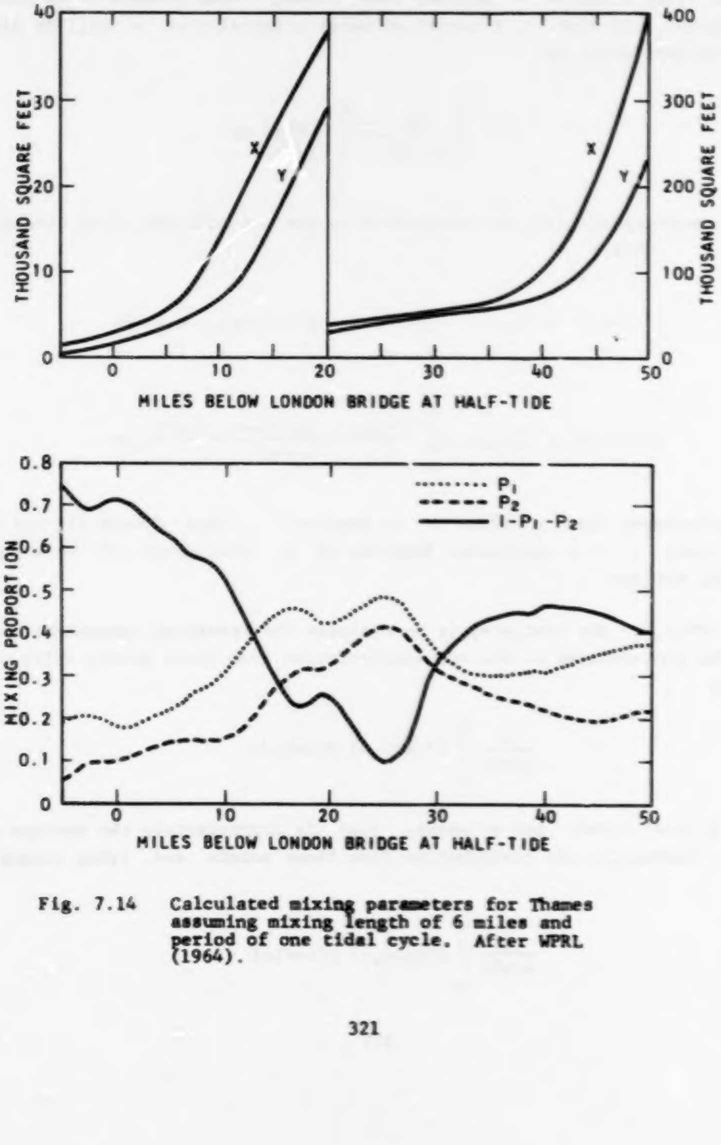


Fig. 7.14 Calculated mixing parameters for Thames assuming mixing length of 6 miles and period of one tidal cycle. After WPRL (1964).

The distribution of substances other than salinity in the Thames is determined by accomplishing the calculation in two parts: the first is the computation of the effect of net displacement due to freshwater discharge, sources of the substance from the periphery of the estuary, and the natural sources and sinks of the substance within the estuary waters; the second is the computation of the effects of tidal mixing. Thus for each time step τ, a substance is represented as being first displaced without tidal mixing, and simultaneously incremented by the cumulative sources and sinks, then mixed without displacement or the effect of source and sink processes. The time step τ must of course be chosen sufficiently small to prevent a degradation of accuracy, and this is dependent upon the reaction rates being sufficiently slow. In the Thames work, τ was on the order of a tidal period.

We denote the concentration of a constituent at position x and time t by $C(x,t)$. Boundary conditions are values of C at the head and mouth of the estuary, and the initial distribution $C(x,0)$ is given. The problem is first to determine $C^*(x,\tau)$, where C^* is the concentration after a period τ without tidal mixing. This problem is pursued from a Lagrangian standpoint. In time t a parcel of water originally at x will be displaced a distance s given implicitly by

$$t = \int_o^s \frac{ds}{u(x+s)} = \int_o^s \frac{A(x+s)}{Q(x+s)}\, ds$$

In addition its concentration will be incremented by the net addition $I(x)$ and source/sink process $-\varphi(C,x,t)$. Thus,

$$C^*(x+s,t) = C(x,o) + \int_o^t \Big[I(x+s) - \varphi(C^*(x+s),x+s,t)\Big]dt$$

or

$$C^*(x+s,t) = C(x,o) + \int_o^s \frac{I(x+s) - \varphi(C^*(x+s),x+s,t)}{u(x+s)}\, ds \tag{7.3}$$

If the total displacement from x after τ is denoted σ, then $C^*(x+\sigma,\tau)$ can be determined from (7.3), and since σ is a continuous function of x, this gives C^* as a function of distance along the estuary.

Given $C^*(x,\tau)$ the next step is to evaluate the resulting concentration $C(x,\tau)$ with tidal mixing. The contribution to the new concentration from those points lying seaward of x is, approximately

$$\frac{1}{A(x)L} \int_o^L C^*(x+\ell,\tau)\, Y(x+\ell)\, d\ell$$

since $Y(x+\ell) = P_2(x+\ell)\, A(x+\ell)$ and we assume $A(x)$ is approximately the average area from $x+\ell-L$ to $x+\ell$. Similarly, the contribution from those points $x+\ell$ lying landward from x $(\ell<0)$ is

$$\frac{1}{A(x)L} \int_{-L}^o C^*(x+\ell,\tau)\, X(x+\ell)\, d\ell$$

Finally, the contribution to the new concentration due to that portion $1-P_1-P_2$ that remains at x is

$$\left[1-P_1(x)-P_2(x)\right] C^*(x,\tau)$$

The new concentration, after mixing, is therefore

$$C(x,\tau) = \frac{1}{A(x)L}\left\{\int_0^L C^*(x+\ell,\tau)\ Y(x+\ell)d\ell + \int_{-L}^{0} C^*(x+\ell)\ X(x+\ell)d\ell \right.$$

$$\left. + LC^*(x,\tau)\left[A(x) - X(x) - Y(x)\right]\right\} \tag{7.4}$$

Equations (7.3) and (7.4) were solved numerically with a spatial increment of two miles. The specific techniques used are straightforward applications of linear algebra so there is no need to review them in detail: Equations (7.1) through (7.4) are sufficient to exhibit the underlying methodology.

2.3.1 Modeling of Temperature Distribution

The temperature as a function of position in the Thames is expressed as the sum of a basic temperature, which is that temperature which would result if there were no heating in the estuary other than natural sources, and a temperature excess. Although the basic temperature can, in theory, be calculated from various meteorological parameters, in the Thames study it was instead calculated by statistical regression equations using the long temperature records available (extending back to the mid-nineteenth century). Regression forms were obtained for stations at Kingston (above the Wier), Greenwich and Crossness, relating the water temperature T_w to the air temperature T_a and to the difference between T_a and its value the preceding month, denoted A. Most of the significant variation was associated with T_a, and all three regression equations were quite similar. For example, the regression form for Greenwich was determined to be

$$T_w = 1.101\ T_a - 0.151\ A + .41 \quad (^\circ C)$$

The basic temperature for the estuary seaward from Crossness was obtained from measured data for the period 1915-1921, which was assumed to be relatively free from artificial heating. This data was expressed in terms of its excess over the temperature at Crossness for the four seasons. Thus a complete longitudinal distribution for the basic temperature was obtained by calculating the temperatures at Kingston, Greenwich and Crossness, passing a smooth curve through these, and extending this curve from Crossness to the mouth using the appropriate temperature difference curves for the season under consideration. Figure 7.15 shows the temperature profiles used to predict the basic temperature along with measured temperatures. The effect of artificial heating in the 1953 example is evident.

The calculation of the temperature excess θ was effected by application of the methodology described in Section 2.3 above. The known sources of heated effluents form the basic input, viz. the expression $I(x)$, and a first-order sink was assumed

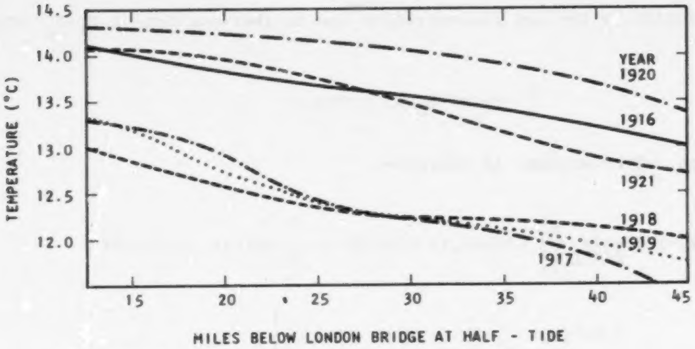


Fig. 7.15(a) Average temperature in Thames seaward of Crossness for April - June quarters of 1916-21. After WPRL (1964).

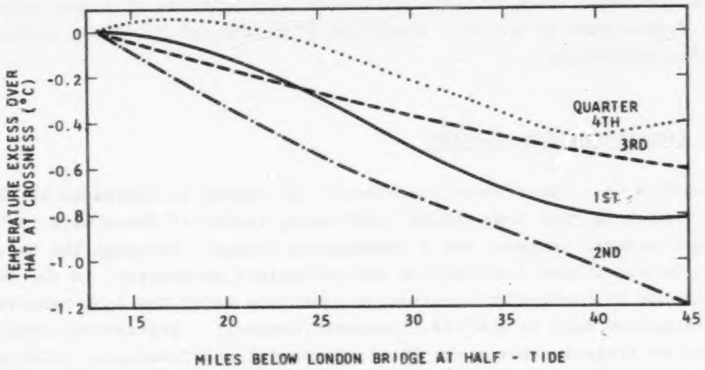


Fig. 7.15(b) Average excess over that at Crossness for same quarter of 1915-21. After WPRL (1964).

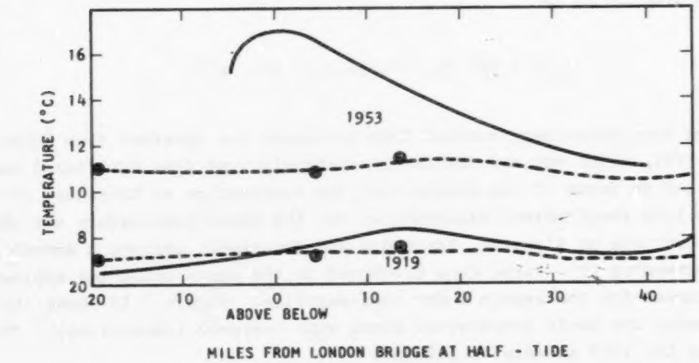


Fig. 7.15(c) Comparison between observed temperature (solid curves) of estuary during October - December quarters of 1919 and 1953 and basic temperature predicted (broken curves and encircled points) for same quarters. After WPRL (1964).

$$\varphi = \frac{g}{z}\,\theta$$

where g is a heat exchange coefficient and z is the depth. The coefficient g was determined from measured data by relating $d\theta/dt$ to the known rate of addition of heat and was found to be 4.0 cm/hr.

2.3.2 Modeling of Dissolved Oxygen Distribution

In the Thames work, the sinks of dissolved oxygen found to be of principal importance are the oxidation of organic carbon and the oxidation of ammonia. The principal sources are reaeration and, in the anaerobic reach, the reduction of nitrates and sulfates. Accordingly, modeling of the DO distribution required modeling of the distributions of carbonaceous demand, organic nitrogen, ammoniacal nitrogen, and nitrates for basic inputs to the DO model.

It was found empirically that the simplest treatment of the carbonaceous demand reasonably consistent with the data was to regard the demand as being the sum of two components: a "fast" constituent and a "slow" constituent, the adjectives referring to the rates of oxidation. The oxidation rate of the "slow" carbon was approximately one-fifth that of the "fast." Therefore, the total carbonaceous oxygen uptake in a sample after a period t becomes

$$X_t = E_c\left[1 - (1-p)\exp(-Kt) + p\exp(-Kt/5)\right]$$

where p denotes the proportion of "slow" carbon in the sample. The value of p depends upon the character of the effluent and was evaluated separately for each major pollutant load on the Thames. Although in several cases it could be assumed that $p = 0$, the value of p in other cases ranged as high as 6/7. E_c is the "effective" total carbonaceous demand, a number somewhat less than the value obtained from stoichiometry by assuming the complete oxidation of all organic carbon. The oxidation rate K was taken to be .234 day^{-1}. The effective demand E_c can be related to the five-day BOD (assuming no nitrification) by setting $t = 5$ days in the above equation, whereupon

$$E_c = \frac{BOD_5}{.69 - .48p}$$

For $p = 0$ this becomes $E_c = 1.45\ BOD_5$. The total carbonaceous demand was obtained by the method of Section 2.3, computing separately the fast and slow demands with a first-order sink with rate $K = .234\ \text{day}^{-1}$ for the fast carbon and $K = .047\ \text{day}^{-1}$ for the slow. The sources $I(x)$ were determined by analysis of effluent data with the above considerations.

The nitrogenous oxygen demand is chiefly due to the oxidation of ammoniacal nitrogen, which is introduced in the estuary both from direct discharges of ammonia and from the hydrolysis of organic nitrogen. Organic nitrogen was assumed to be hydrolysed at the same rates as the organic carbon; it was therefore represented as the sum of a "fast" and a "slow" organic nitrogen exactly as the carbonaceous demand was treated. As only the fraction E_c/U_c of the total organic carbon is effectively oxidized (where U_c is the theoretical oxygen demand for the total oxidation of the organic carbon, so that $U_c = 2.67$ C), the ammonia produced from the hydrolysis of organic nitrogen is $E_c N_{org}/U_c$, where N_{org} is the content of organic nitrogen in a particular effluent. The sum of the fast and slow organic nitrogen distributions becomes a source in the ammoniacal nitrogen equation. Ammonia was assumed to decay according to a simple first-order expression with rate constant $\kappa = .102\ \text{day}^{-1}$ at 20°C when the DO concentration is greater than 5%. When the DO concentration falls to 5% of saturation, nitrification was considered to proceed at a reduced rate (see below) so as to maintain the DO at 5% as long as possible. If the oxidation of organic carbons is sufficient to drive the DO below 5% of saturation, even in the absence of nitrification, then nitrification was assumed to cease, and the reduction of nitrates to occur and thereby maintain the level of DO at 5% of saturation.

In addition to effluent discharges and freshwater inflows, nitrates are introduced into the estuary as a result of the oxidation of ammonia. Except for those reaches in which the DO is at 5% of saturation and nitrification has ceased, nitrates were considered to be inert. For convenience the nitrate was expressed as the equivalent oxygen produced in the reduction (to nitrogen) of the nitrate, and thus available for oxidation of the organic carbon. This is five-eighths the amount of oxygen required to produce the same amount of nitrate by oxidation of ammonia.

The source of oxygen by diffusion from the atmosphere was represented by the classical expression

$$\frac{f}{z} D$$

where z is the depth, D is the oxygen deficit, and f the exchange coefficient. For the Thames work, it was concluded that a value of $f = 5.0$ cm/hr throughout the estuary was sufficiently accurate for initial calculations. (See Section 2.4 and Table 7.3.)

Calculation of a DO profile is accomplished by first computing the carbonaceous BOD (the sum of the "fast" and "slow" demands) and the nitrogenous demand assuming aerobic conditions, i.e. that nitrification occurs at the unrestricted rate κ. The distribution of nitrate is obtained assuming production through the oxidation of ammonia and the contributions from various discharges, but no sinks of nitrate in the watercourse. The resulting DO deficit due to the combined sinks of carbonaceous and nitrogenous oxidation is calculated. The temperature profile is a basic input to this calculation in that it affects the solubility of oxygen and the reaction rates of the biochemical oxidation processes. If the resulting deficits are less than $.95\ C_s$ (C_s denoting the saturation concentration of DO) then the resulting profile is the final solution. If, however, there are reaches in which $D > .95\ C_s$, the profile must be recomputed with allowance made for anaerobic processes. This is performed by an essentially trial-and-error technique. The carbonaceous demand profile is assumed to be correct, whatever the DO concentration may be, therefore it is not modified. However, the ammonia concentration will have been underestimated in certain reaches because, in fact, restricted nitrification should have been assumed. Therefore, a function $U(x)$ is added to the ammonia concentration to compensate for this error; the nitrate equivalent $-\frac{5}{8} U(x)$ is added to the nitrate concentration to correct for the overestimation of nitrates. $U(x)$ is determined by trial calculations of the deficit profiles. There is an obvious upper limit to the value of $U(x)$, namely the total increase in nitrate (at x) due to nitrification, and setting $U(x)$ equal to this maximum is equivalent to specifying no nitrification, i.e. $\kappa = o$. Even with no nitrification, it is evident that there may remain reaches in which the deficit still exceeds $.95\ C_s$. For these areas, nitrate reduction is assumed, so that the concentration of nitrates is further reduced by the addition of the function $-V(x)$, which is also determined by trial-and-error. The maximum permissible value of $V(x)$ is that value which reduces the total nitrates to zero. Should there still remain reaches with deficit in excess of $.95\ C_s$ and for which the nitrate concentration is zero, the deficit profile is further modified by a function

-W(x) representing the reduction of sulfates. The maximum value of this function is that which balances the carbonaceous demand, i.e. that which brings the DO concentration up to zero.

The finite-difference solution to the relevant equations was performed using 35 points along the estuary at 2 mile intervals beginning at Teddington Wier. In general, the solutions obtained were for steady-state conditions, so that the calculations were advanced in time with constant inputs until an equilibrium solution resulted. For boundary conditions at the mouth of the estuary it was assumed that the concentrations of polluting substances were zero. At the head, the concentrations of the polluting substances were measured values or (for predictions) estimated values. For dissolved oxygen, the sampling point furthest up the estuary was below the River Brent at Kew, some 6 miles below the head of the estuary. Accordingly, the boundary value for DO at the Wier was taken to be that value which brought the model value at Kew into agreement with the measured value.

2.4 MODEL RESULTS

2.4.1 Calculated Profiles and their Accuracy

The methods described in Section 2.3 *et seq.* were applied to calculations of the profiles of DO and organics using measured flows and loadings for the period 1950-1961 and the computed results were compared with observed concentrations in the estuary. Calculations were performed by dividing each year into quarters, averaging the inputs (inflows and loadings) over each quarter, and obtaining the steady-state profiles for these averaged inputs. These results were then compared with the averaged empirical data for that quarter.

Figures 7.16 and 7.17 are examples of the intermediate calculations of temperature, and organic carbon and nitrogen (oxygen equivalent), respectively. Both the calculated and observed temperature profiles are shown in Figure 7.16, as well as the computed basic distribution, i.e. that profile which would result in the absence of artificial heating. In Figure 7.17, the calculated organic carbon and nitrogen are separated into their "fast" and "slow" components.

Figure 7.18 displays the results of calculations for 1951, 1953, 1954, 1957, 1960 and 1961 for the parameters dissolved oxygen, ammoniacal nitrogen, and oxidized nitrogen (nitrates). Much of the discrepancy in the DO profiles was found to be attributable to large variations in the inflow during the quarter, hence producing significant departures from the assumed steady state. This was partially compensated for by subdividing the quarter into thirteen weekly records, averaging the inflows for each week and computing the resulting steady-state solution. The thirteen profiles so obtained were then averaged to arrive at a revised quarterly average. Although no allowance was made for week-to-week variations in the loadings of temperatures, nor for smaller time scale variations in inflow, this calculation produces noticable improvements in the refined profiles. Note, for example, the results for 1954 of Figure 7.18. The change in temperature due to the same kind of averaging is demonstrated by Figure 7.19 (cf. Figure 7.16).

Figure 7.20 shows the predicted and observed profiles of DO obtained by averaging by quarters the empirical concentration for the period 1950-1955 and by averaging the corresponding predictions after allowance is made for weekly variation in freshwater inflow. The systematic discrepancies between observations and predictions suggested that a seasonal variation

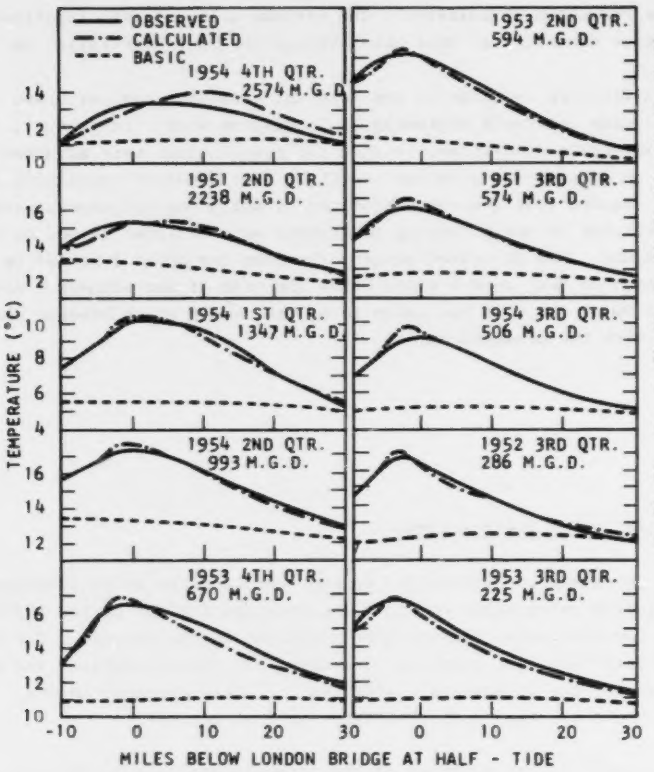


Fig. 7.16 Examples of computed and observed temperature distributions in the Thames. Heat exchange coefficient taken to be 3.7 cm/hr. Average flows at Teddington are indicated. After WPRL (1964).

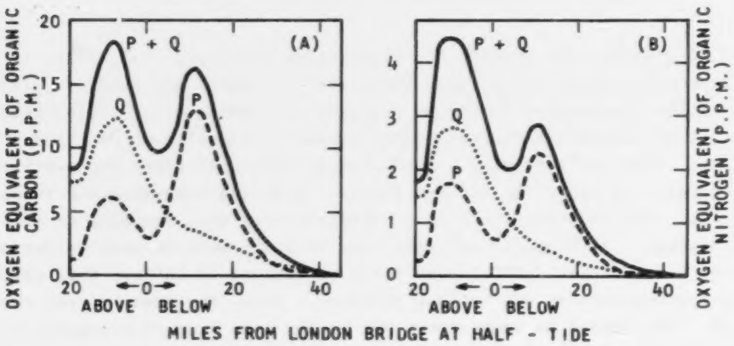


Fig. 7.17 Example of calculated distribution of organic carbon oxygen demand and organ. nitrogen distribution (oxygen equivalent). P indicates "fast" oxidation-hydrolysis rate: Q indicates "slow." After WPRL (1964).

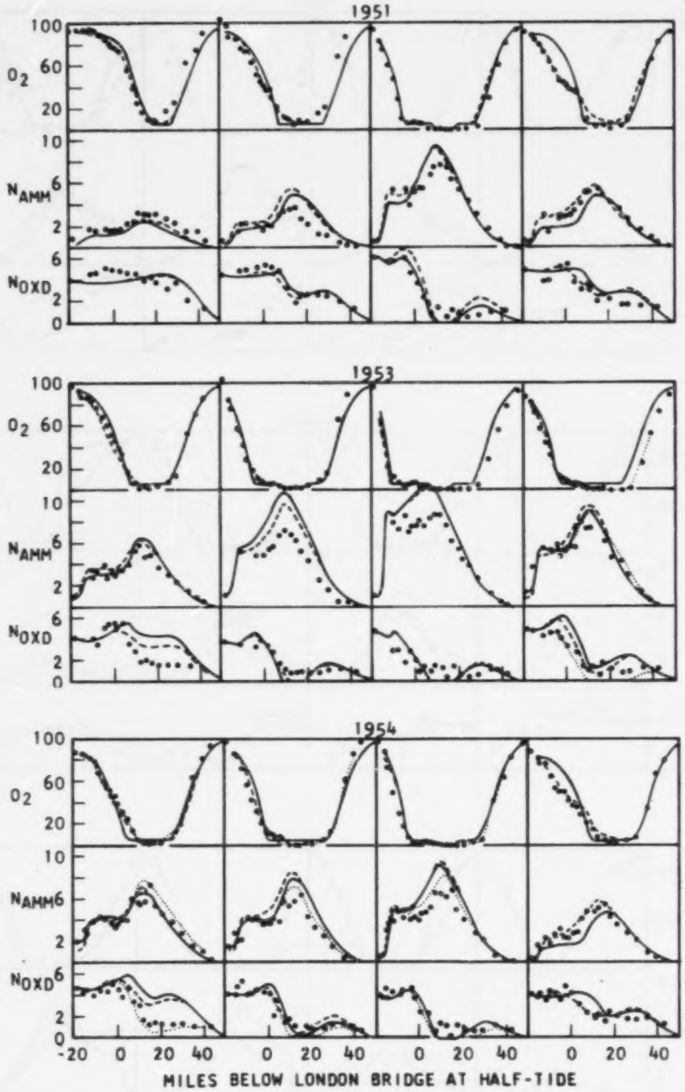


Fig. 7.18 **Examples of Calculated DO, Ammonia (N_{amm}) and Nitrates (N_{oxd}) Profiles Compared with Measured Data.**

First through fourth quarters of each year beginning with the first (January-March) at left.

Solid curves: Calculated
Broken curves: Calculated profiles with variation of inflow
Plotted points: Measured concentrations (London County Council data)
Dotted curves: W.P.R.L. data

DO in percent saturation, N_{amm} and N_{oxd} in p.p.m.
After WPRL (1964).

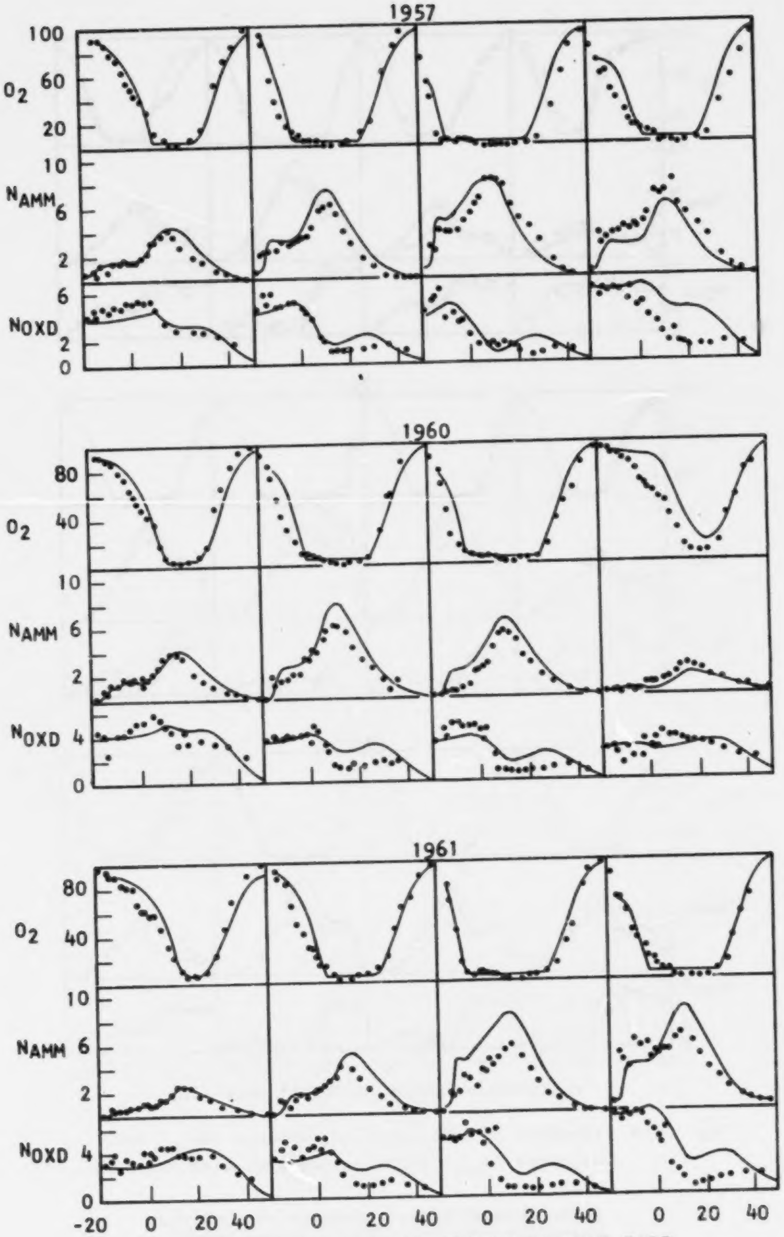


Fig. 7.18 Continued.

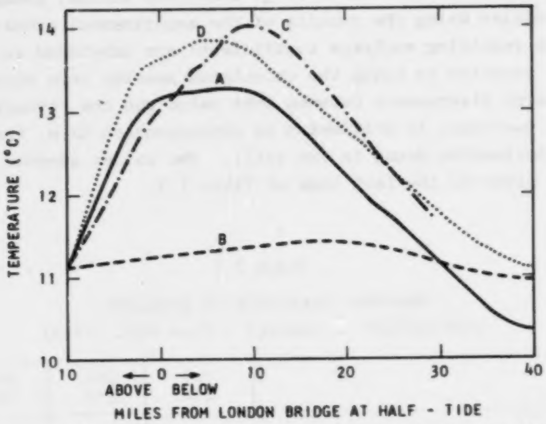


Fig. 7.19 Effect of variations in fresh-water flow during quarter on predicted temperature distribution (for fourth quarter of 1954). A, observed; B, basic; C, predicted to be in equilibrium with mean flow during quarter; D, predicted allowing for variations in flow during quarter. After WPRL (1964).

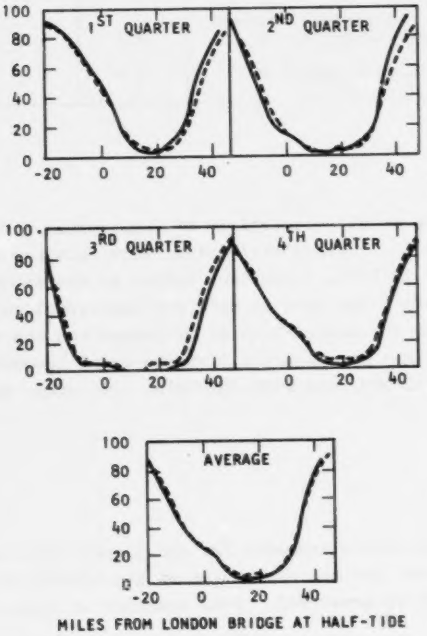


Fig. 7.20 Observed and predicted DO profiles (per cent saturation) in Thames for corresponding quarters of 1950 to mid-1955, and for entire period. Solid curves, observed data. Broken curves, calculated. After WPRL (1964).

in the exchange coefficient might be in evidence. On the basis of extensive field and laboratory investigations, the parameters most important to the value of the exchange coefficient f were found to be temperature, contaminants (e.g. dissolved solids, sewage, surface impurities), and wind. f was modified using the results of the experimental studies (some of which were quite tentative). The resulting exchange coefficients are tabulated in Table 7.3. In comparison, the value of f required to bring the calculated results into agreement with the observed is also shown. The large discrepancy between this value and the "theoretical," particularly in the second and fourth quarters, is attributed to phytoplankton (i.e. increased photosynthesis in the spring and phytoplankton decay in the fall). The values adopted for f for use in model predictions are given in the last line of Table 7.3.

TABLE 7.3

SEASONAL VARIATION IN EXCHANGE COEFFICIENT f (cm/hr) , From WPRL (1964)

	1st Qtr.	2nd Qtr.	3rd Qtr.	4th Qtr.
Expected values of f from experimental work with allowance for seasonal variation in:				
(a) temperature	4.5	5.1	5.5	4.9
(b) temperature and contaminants	5.0	4.8	5.1	5.0
(c) temperature, contaminants and wind	5.4	4.7	4.8	5.1
Calculated from discrepancy between observed and predicted DO	5.3	5.5	4.2	4.3
Final values used in predictions	5.2	5.3	4.3	4.5

The effects on the model calculations of temperature and inflow for the four seasons are evident from Figure 7.21. These distributions were obtained by assuming the polluting loads to be the average for 1951-54, a constant inflow in the indicated amount, and a constant temperature along the estuary. The plotted data are individual measurements from the period 1951-54 grouped according to the temperature at Crossness and the flow at Teddington. The data were sorted by temperature into groups ±2½°C from the model temperatures and into the flow ranges 400-600 MGD, 1250-1750 MGD, and 2500-3500 MGD. All other data for the period were excluded.

2.4.2 Model Application

The principal application intended for the Thames model was to serve as an aid to management in providing a tool for the evaluation of the effects of various outfalls and for the evaluation of management alternatives. Some examples of these types of applications are given in this section.

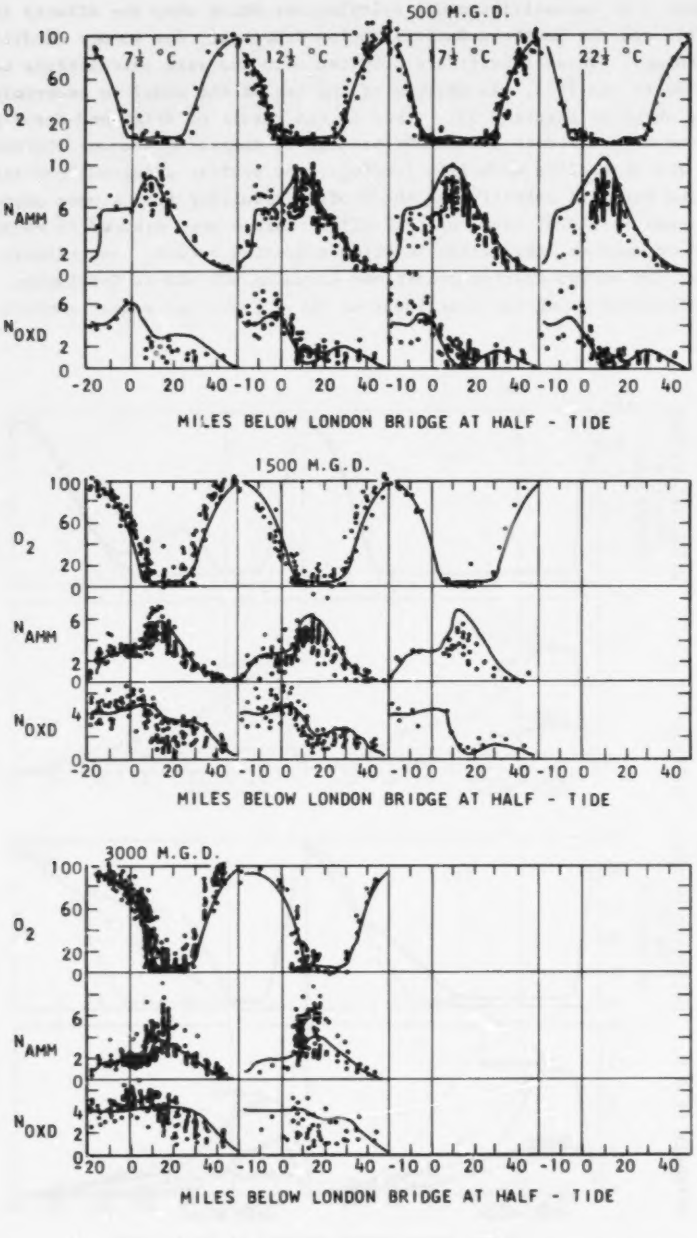


Fig. 7.21 Observed and calculated effects of temperature and fresh-water flow on distributions of dissolved oxygen (per cent saturation), ammoniacal nitrogen (p.p.m.) and oxidized nitrogen (p.p.m.). Solid curves, calculated distributions for average polluting loads in 1951-54, and flows at Teddington and temperatures as indicated. Plotted Points, observed concentrations. After WPRL (1964).

Figure 7.22 exemplifies model calculations which show the effects of relocating the Northern Outfall and the Southern Outfall (below Crossness) for summer conditions and estimated 1964 loadings. These results are compared with the same calculations using the average loadings of 1950 to mid-1955. An example of the use of the model to ascertain required treatment levels is shown in Figure 7.23. This is the result of trial-and-error determination of level of treatment required to permit the passage of migrating salmon. Curves A, B, and C are, respectively, the DO profile with 1964 loadings, the profile obtained from assuming secondary treatment at the Northern Outfall, and the profile resulting from a more extensive reduction in polluting loads (see WPRL 1964, pp. 527-528). Salmon were assumed to require 30% saturation during the second quarter, the period in which migration occurs. Accordingly, curves A, B, and C were obtained for second quarter conditions assuming 400 MGD at Teddington. In comparison, curve D was calculated using the same loads as curve C but for summer conditions with 170 MGD at Teddington.

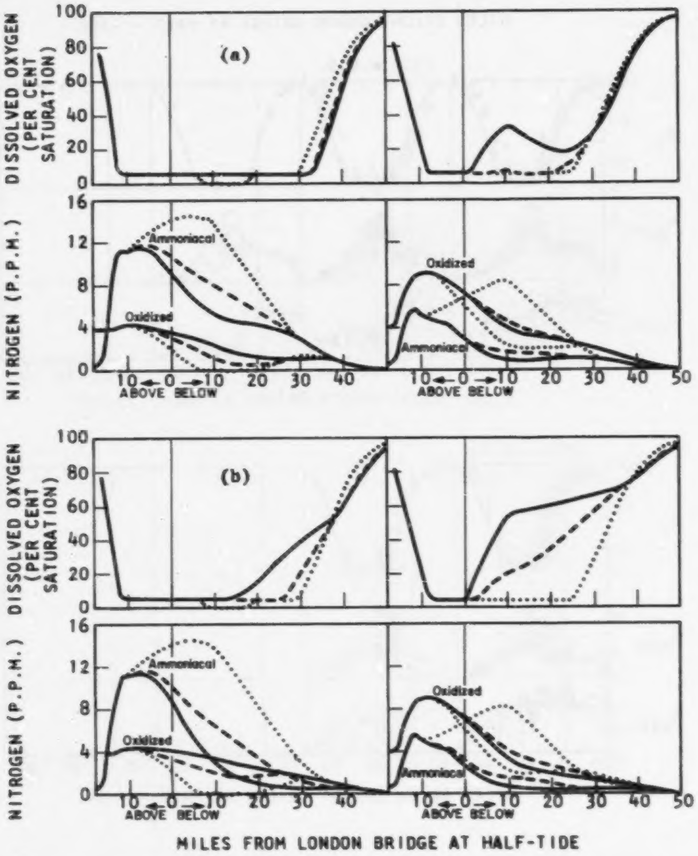


Fig. 7.22 Effect of moving discharge points to (a) 30 miles, and (b) 40 miles below London Bridge. Outfalls in present position (dotted), Northern Outfall relocated (dashed), Northern and Southern Outfalls relocated (solid). Average loadings for 1950-55 (left) and estimated loadings for 1964 (right). After WPRL (1964).

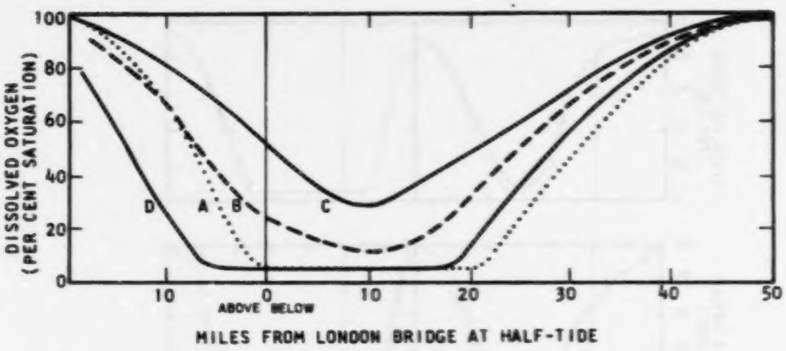


Fig. 7.23 Calculated DO profiles assuming various loading conditions in estuary (see text). After WPRL (1964).

The period 1950-1961 is of interest in demonstrating the efficacy of the Thames model for predicting the results of improved treatment due to various alterations at the Northern Outfall Works. For the period 1950 through mid-1955, the polluting loads at the Northern Outfall were relatively constant, discharging 190 MGD of which 21% received secondary treatment. In mid-1955, a new sedimentation plant became operable, thereby reducing the load. From then until 1960, the average flow was 195 MGD of which 18% received secondary treatment. Beginning in 1960, a new aeration plant was operated further reducing the load, and through 1961 the average flow was 212 MGD with 45% given secondary treatment. Model calculations were performed for the first and third quarters using the average loads and temperatures for these three periods. Empirical curves for the same three periods were obtained from observed data (using the interpolation scheme to "normalize" the inflows) and compared to the predictions. The observed and predicted DO profiles are shown in Figure 7.24, and the corresponding ammoniacal nitrogen and nitrates are shown in Figure 7.25. The predicted curves only take into account the variations in loads at the Northern Outfall; all other changes in polluting loads are neglected. In the vicinity of the Northern Outfall (mile point 11) this is not important, but elsewhere, particularly upstream, the effects of other sources can become significant. The large observed changes in DO above the Bridge were attributed to such variations in the loads.

Extensive predictions were made of the quality in the Thames to be expected in 1964. At the time of issuance of the report on the Thames work (WPRL 1964), extensions and modifications in two of the larger municipal treatment plants, Southern Outfall and Mogden, were underway and scheduled for completion in 1964. The effects of these changes were incorporated in the predictions by employing the expected effluent characteristics. In addition, increased discharge in the Northern Outfall (above the River Roding), and some diversion of wastes through the Northern Outfall were also considered. Figure 7.26 shows the results of the model calculations for the worst case of summer conditions and low inflow (the legislated minimum). For comparison, curves derived from empirical data for 1920-29 and 1950-59 are shown. These curves were obtained by compensating the observed measurements for variation in flow using empirical "rating curves." In contradistinction, Figure 7.27 displays the same curves for

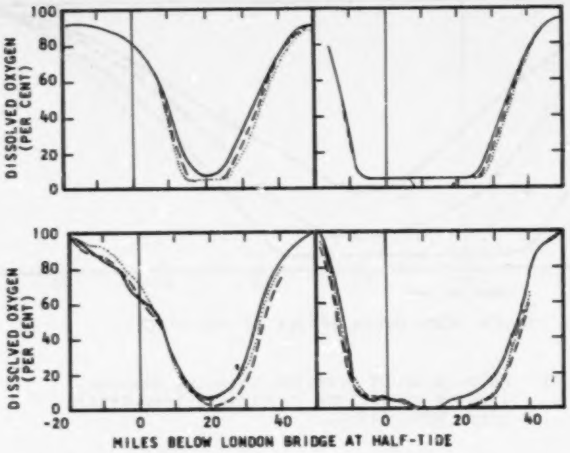


Fig. 7.24 Predicted (above) and observed (below) DO profiles during first quarter (left) and third quarter (right), following improvements in treatment at Northern Outfall. 1961 (solid), mid-1955 to 1959 (dashed), 1950 to mid-1955 (dotted). After WPRL (1964).

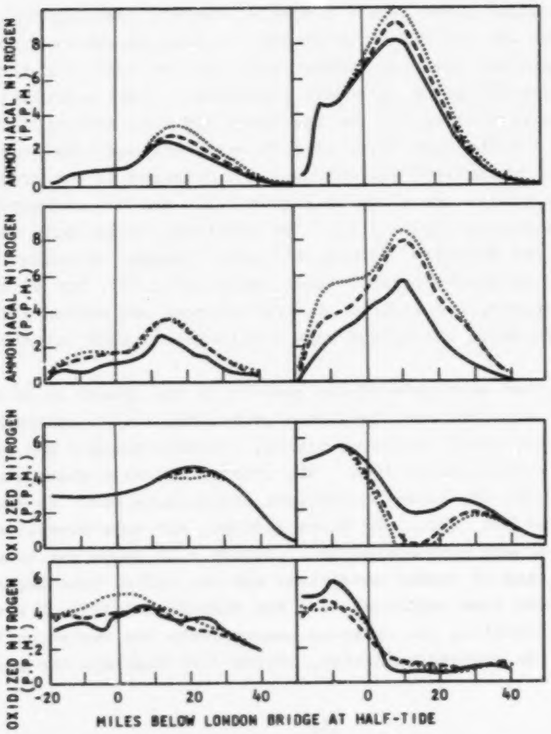


Fig. 7.25 Ammoniacal and oxidized nitrogen profiles corresponding to DO profiles of Fig. 7.24. After WPRL (1964).

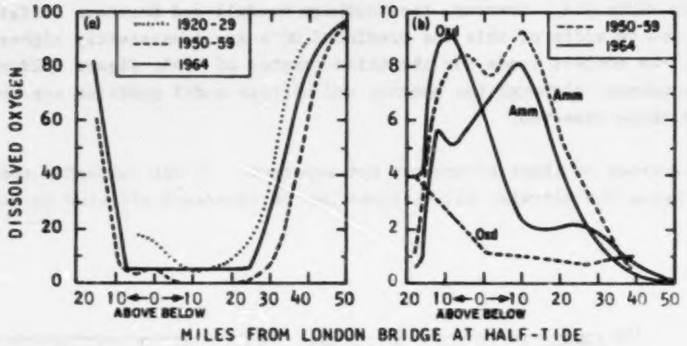


Fig. 7.26 Predicted profiles of DO, Ammoniacal Nitrogen and Oxidized Nitrogen for third quarter (summer) conditions, 170 MGD flow at Teddington, and estimated loads for 1964. Broken curves are derived from observed data for indicated periods. After WPRL (1964).

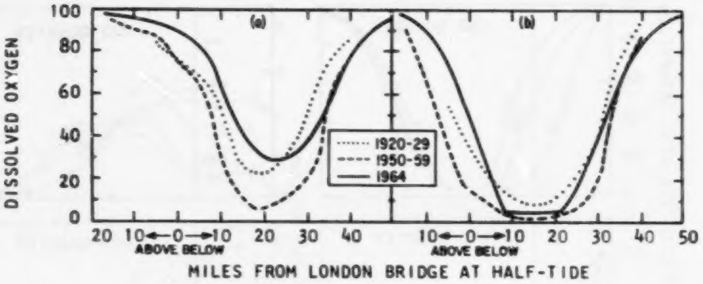


Fig. 7.27 Predicted profiles of DO for 1964 loadings with profiles obtained from observed data. (a) First quarter, inflow 4000 MGD at Teddington. (b) Second quarter, inflow 1200 MGD at Teddington. After WPRL (1964).

different seasons and inflows. In Figure 7.28 are given the steady-state predictions for 1964 for all four quarters under various inflows. For these predictions and those of Figures 7.26 and 7.27, the exchange coefficient was assumed to vary seasonally as specified in Table 7.3.

It is of particular interest to compare these predictions with the concentrations actually measured after the improvements in the Mogden and Southern Outfall plants were completed. In Gameson and Hart (1966) this comparison was made using data from both 1964 and 1965, and is displayed in Figure 7.29. The model results were obtained from the predictions of Figure 7.28 by interpolation to the measured inflows. The comparison is somewhat disappointing overall. Lack of agreement in DO values in the upper reach can be attributed to the fact that the Mogden load was in fact much larger than the load used in the predictions, as indicated in Table 7.4. However, the Southern Outfall and Northern Outfall BOD loads were overestimated and in spite of this the predicted DO's are consistently higher than the measured values. Using the correct loads for the third quarter of 1964, Figure 7.29(a), did not improve the DO correspondence, although the ammonia and nitrate model profiles are brought into better agreement with those observed.

The sources of these errors are not apparent. It was suggested that the ammonical nitrogen, and hence the nitrate, calculations may be adversely affected by using what appears

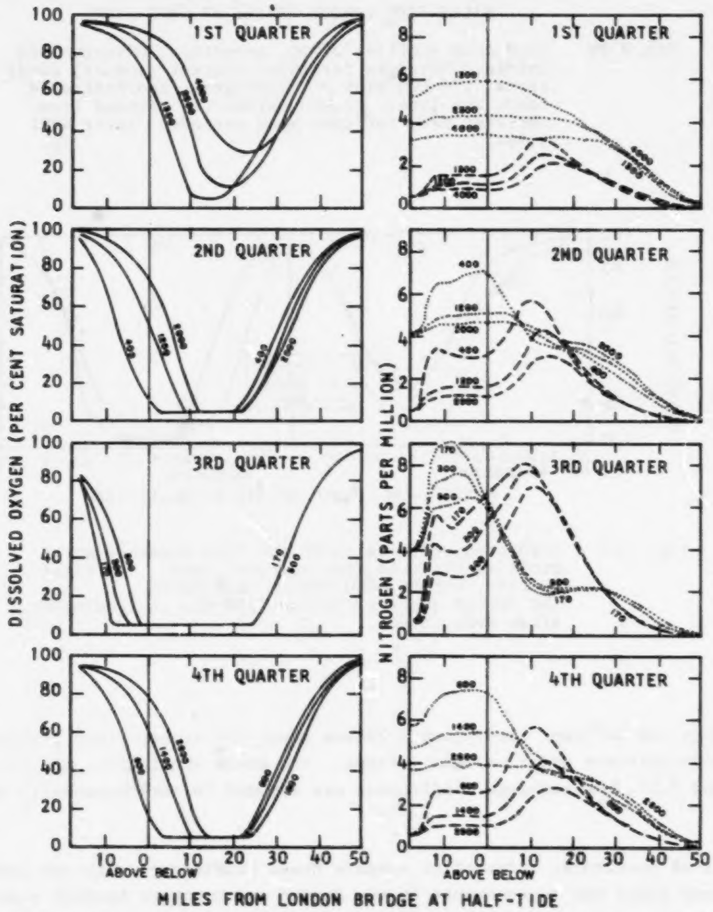
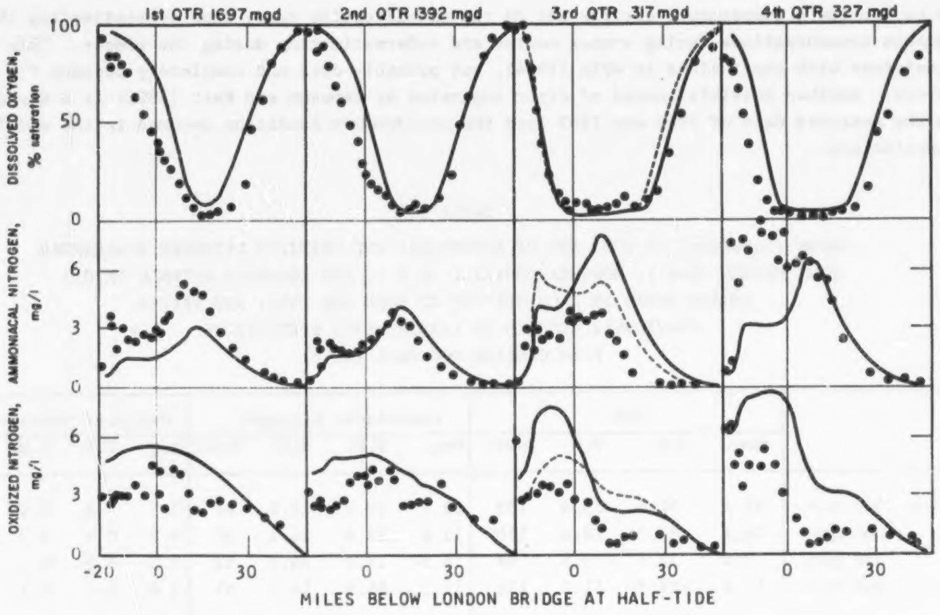
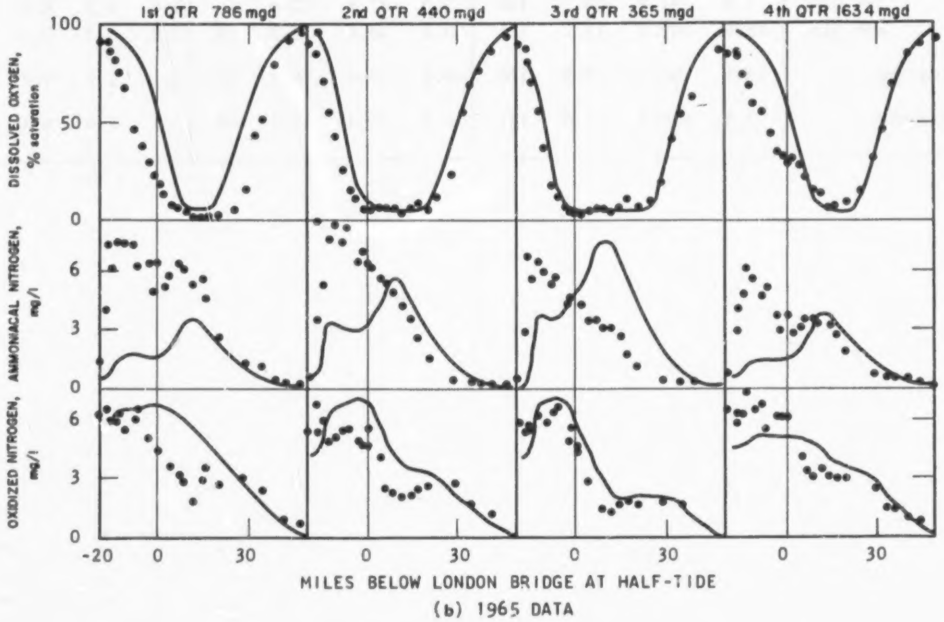


Fig. 7.28 Predicted profiles of DO (solid), ammoniacal (dashed), and oxidized (dotted) nitrogen for estimated 1964 loads. Flows at Teddington in MGD are shown. After WPRL (1964).



(a) 1964 DATA



(b) 1965 DATA

Fig. 7.29 Observed concentrations of DO, Amm. N and Nitrates compared with profiles predicted from assumed loads (Table 7.4). Broken curves in (a) are the profiles predicted from the measured loads. After Gameson and Hart (1966). Data collected by Greater London Council.

to be too low a temperature coefficient on the nitrification rate, thus overestimating the ammonia concentrations during summer months and underestimating during the winter. This is consistent with conclusions in WPRL (1964), but probably does not completely account for the errors. Another possible source of error suggested by Gameson and Hart (1966) is a departure in the measured data of 1964 and 1965 from the steady-state condition assumed in the model computations.

TABLE 7.4

LOADS (tons/day) OF BOD, AND OF AMMONIACAL AND OXIDIZED NITROGEN DISCHARGED FROM MOGDEN (Mog.), NORTHERN OUTFALL (N.O.), AND SOUTHERN OUTFALL (S.O.) SEWAGE WORKS IN EACH QUARTER OF 1964 AND 1965, AND VALUES PREVIOUSLY ASSUMED IN LABORATORY'S PREDICTIONS
From Gameson and Hart (1966)

	BOD				Ammoniacal Nitrogen				Oxidized Nitrogen			
	Mog.	N.O.	S.O.	Total	Mog.	N.O.	S.O.	Total	Mog.	N.O.	S.O.	Total
1964, 1st Qtr.	27.1	90.9	15.4	133	11.7	23.9	12.6	48	0.5	1.4	0.4	2.3
2nd Qtr.	16.1	83.3	10.4	110	11.6	22.6	16.1	50	0.7	0.6	0.3	1.6
3rd Qtr.	6.4	72.5	9.8	89	8.9	19.2	14.0	42	1.5	0.5	0.2	2.2
4th Qtr.	11.6	108.5	11.3	131	11.2	24.9	14.5	51	1.0	0.5	0.1	1.6
1965, 1st Qtr.	12.3	105.7	14.6	133	11.2	25.5	14.7	51	0.2	1.1	0.1	1.4
2nd Qtr.	11.4	98.4	15.7	126	10.7	20.6	14.5	46	0.1	1.0	0.1	1.2
3rd Qtr.	7.8	91.2	10.7	110	8.8	17.6	13.4	40	2.4	1.2	0.2	3.8
4th Qtr.	12.6	103.1	15.1	131	9.6	19.4	14.2	43	2.0	3.5	0.3	5.8
Average	13.1	94.2	12.9	120	10.5	21.7	14.2	46	1.1	1.2	0.2	2.5
Assumed	3.8	110.5	17.0	131	6.1	24.1	16.2	46	5.7	1.4	nil	7.1

3. THE DECS MODEL

One of the most important and comprehensive estuarine management studies to have been undertaken in this country was that performed by the FWPCA in cooperation with the Delaware River Basin Commission and various state and local agencies in Pennsylvania and New Jersey, viz. the Delaware Estuary Comprehensive Study (DECS). The overall objectives of this study included the following (FWPCA 1966):

(i) determine the cause and effect relationships between pollution from any source and the deteriorated quality of water in the estuary;

(ii) develop methods of water quality management including the development of techniques of forecasting the variations in water quality due to natural or man-made causes;

(iii) prepare a comprehensive program for the improvement and maintenance of water quality in the estuary including the waste removals and other control devices necessary to manage the quality of water in the estuary for municipal, industrial and agricultural water use, and for fisheries, recreation, and wildlife propagation.

The modeling approach employed in this study was the application of the technique of finite differences to the steady-state and time-dependent (tidal-averaged) conservation of mass equations. (Several program codes therefore exist, corresponding to the steady-state and time-varying models in various stages of evolution, but since their unifying feature is the one-dimensional segmentation for finite-difference solution, these programs are referred to collectively as the DECS model throughout this chapter.) As the details of the model are well-documented (Thomann 1963, Pence et al. 1968, Jeglic and Pence 1968, and see Chapter III, Sections 3 and 5), it is the purpose of this section to review its application. The model has not only been applied fruitfully to the Delaware Estuary but to other estuaries as well. In particular, quite extensive application has been made to the Potomac, and the model was adapted for two-dimensional computations for use on Hillsborough Bay.

3.1 THE DELAWARE ESTUARY

The Delaware, which drains the vast Pennsylvania-New Jersey urban development, is one of the most important estuaries on the New England Seaboard. The estuary serves the Pennsylvania-New Jersey area as a source for municipal water and as receiving water for the wastes of the urban complex. The latter has resulted in seriously degraded water, so that quality in the Delaware has become a problem of increasing magnitude in recent years. Recreational uses of the estuary have been seriously truncated. The commercial yield of shad, sturgeon, white perch and a number of other finfish has declined to the point of being economically negligible. (This, of course, is not solely attributable to degraded water quality. Also, in contrast, the menhaden has become of great economic importance, due to broadening industrial application of the catch.)

3.1.1 Characteristics of the Estuary

The Delaware River extends from its headwaters in the south-central area of New York State to the Atlantic Ocean at the coastal limits of Delaware and New Jersey. The estuarine area is the reach between Trenton, N. J., and the ocean (see Figure 7.30), and the Delaware Estuary Comprehensive Study was principally concerned with 86 miles of the river between Trenton and Liston Point. Figure 7.30 shows the segmentation employed in the DECS model. (These sections offer a convenient means of referring to specific reaches of the estuary and will be used for this purpose hereafter.) The estuary at the ocean has a total drainage area of approximately 13,500 square miles. The major tributary to the Delaware Estuary is the Schuylkill River which joins the main stream in the vicinity of Philadelphia. The mean annual discharges of the Delaware and Schuylkill Rivers are on the order of 12,000 cfs at Trenton and 3,000 cfs at Philadelphia, respectively. The total length of the Delaware Estuary between Trenton and the limit at Capes May and Henlopen is approximately 135 miles.

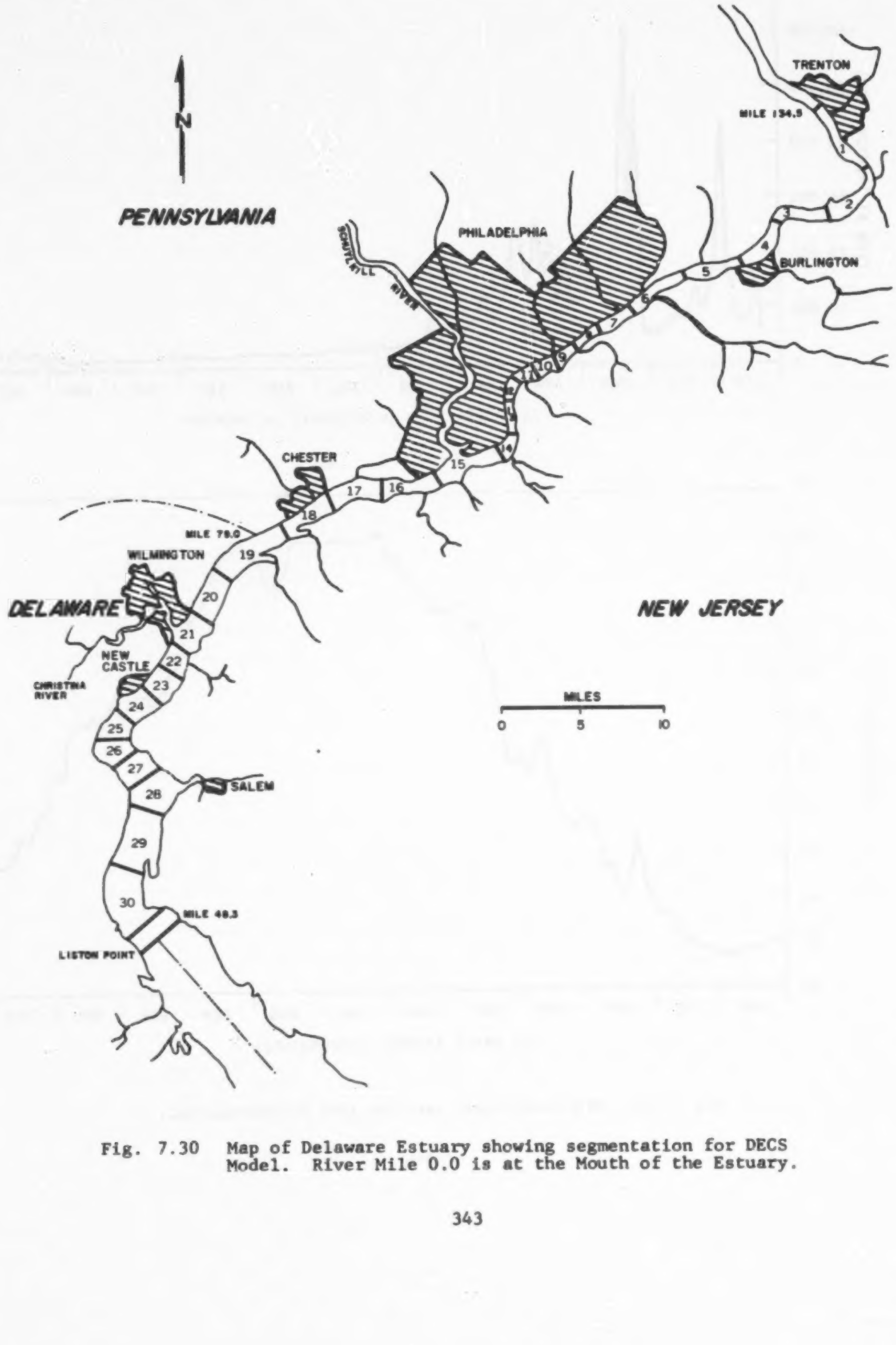
Tidal elevation changes in the Delaware River are observed from the mouth to Trenton. Mean water stage varies from a minimum of 5.5 feet at Reedy Point to a maximum of 6.8 feet at Trenton under average flow conditions. Tidal current reversals occur along the river above Burlington, approximately 10 miles below Trenton. Average maximum current velocities within the estuary are approximately 3.0 fps. The Schuylkill River exhibits tidal stage changes and current reversals to the location of the Fairmount Dam, eight miles above its mouth. Salinity intrusion in the Delaware Estuary generally extends to the area between Wilmington and Marcus Hook for mean freshwater discharge conditions, although during drought periods significant chloride concentration is observed near Philadelphia.

Waste discharges to the Delaware Estuary are both municipal and industrial in origin, with the municipalities generally representing the largest waste sources. The spatial distribution of discharged loads in 1964 is exhibited in Table 7.5. In general, the water quality at the head of tide at Trenton is good, but begins to deteriorate downstream. From Torresdale, Pa., Segment 7 (see Figure 7.30), to below the Pennsylvania-Delaware state line, Segment 19, the deterioration is extreme; as a result of waste discharges, dissolved oxygen is almost completely depleted in some locations and production of gases from anaerobic organic deposits occasionally occurs. The concentration of coliform bacteria resulting primarily from unchlorinated municipal wastes is very high in the same stretch of river. Acid conditions due to industrial waste discharges have been observed for several miles above and below the Pennsylvania-Delaware state line.

3.1.2 Model Application and Results

An extensive comparison has been made of observed DO concentrations of 1964 with DO concentrations computed from the DECS model (Pence et al. 1968). The Delaware was segmented, as indicated in Figure 7.30, into thirty sections each of which was assigned a (mid-tide) volume and cross-sectional areas at the junctions from physiographic data of the Corps of Engineers. Basic inputs were the river flows measured at Trenton and water temperatures measured by the USGS. Water temperature was assumed to be uniform throughout the estuary but to vary with time. Plots of water temperatures and inflows with time are given in Figure 7.31.

The average carbonaceous loads for 1964 (Table 7.5) were used in the DECS calculations. The decay rate for carbonaceous BOD was taken to be .23 day^{-1} at 20°C. Nitrogenous


N
PENNSYLVANIA
TRENTON
MILE 134.5
PHILADELPHIA
SCHUYLKILL RIVER
BURLINGTON
CHESTER
MILE 79.0
WILMINGTON
DELAWARE
NEW JERSEY
NEW CASTLE
CHRISTINA RIVER
SALEM
MILE 48.3
LISTON POINT
MILES
0
5
10
1
2
3
4
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11
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13
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17
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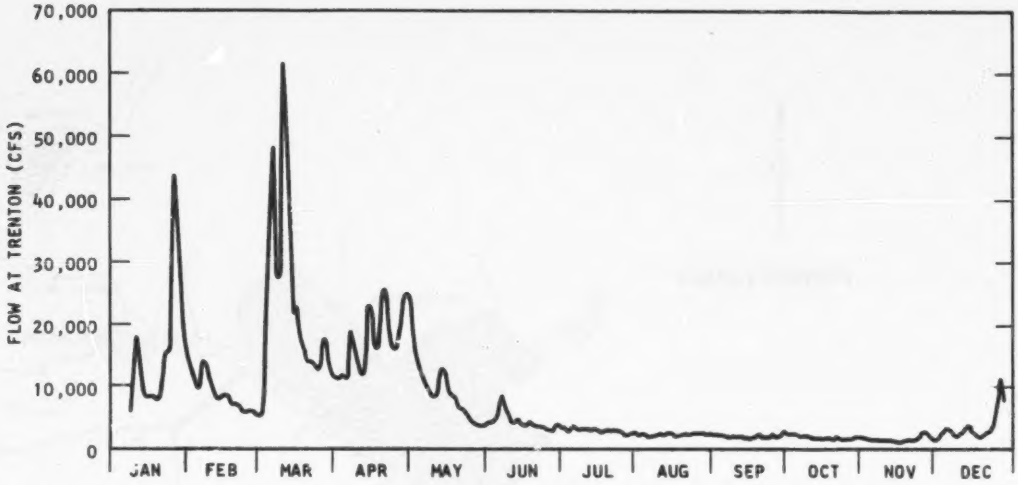
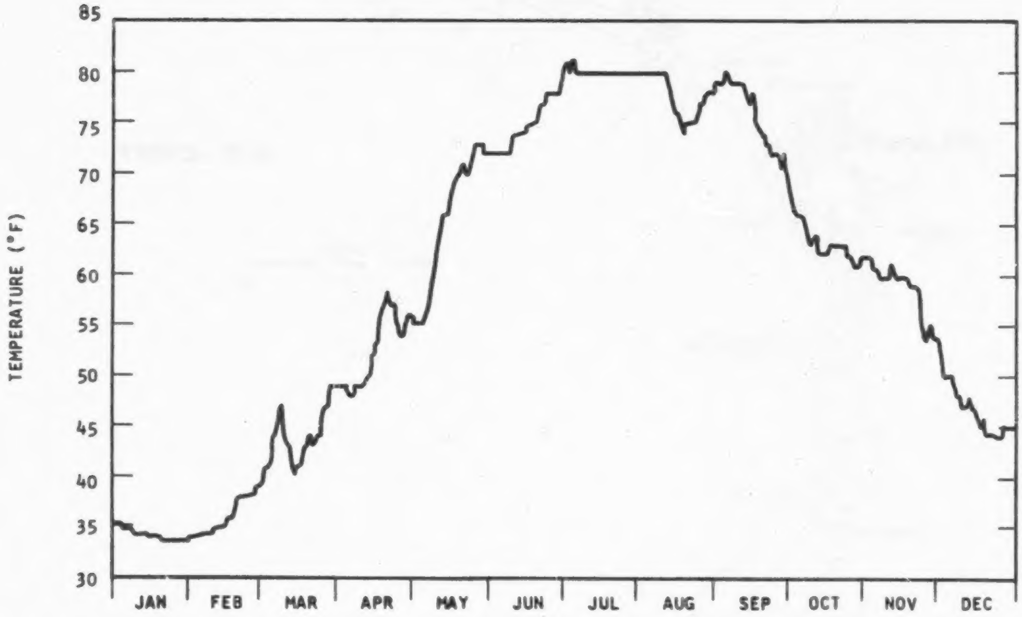
Fig. 7.30 Map of Delaware Estuary showing segmentation for DECS Model. River Mile 0.0 is at the Mouth of the Estuary.



(a) RIVER FLOW IN DELAWARE AT TRENTON



(b) DAILY AVERAGE TEMPERATURES

Fig. 7.31 DECS model input data for 1964 DO calculations.

TABLE 7.5

1964 Waste Loading in the Delaware Estuary
Pounds Per Day of Carbonaceous Biochemical Oxygen Demand

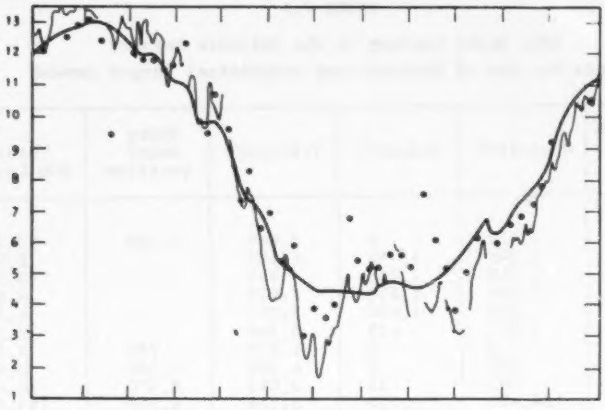
Section (Fig. 7.30)	Municipal	Industry	Tributary	Storm Water Overflow	Total BOD Load
1	3,570	0	2,869	1,360	7,799
2	2,100	2,750	4,107		8,957
3	3,380	1,635	982		5,997
4	2,720	2,850	1,078		6,648
5	900	1,400	2,047		4,347
6	1,075	435	5,798		7,308
7	0	0	1,875	230	2,105
8	520	0	4,309	1,580	6,409
9	795	35	3,095	8,570	12,496
10	128,610	7,550	3,146	4,390	143,695
11	720	1,570	3,189	16,780	22,259
12	0	0	1,105	4,480	5,585
13	62,080	13,925	1,800	7,410	85,215
14	174,520	19,670	1,566	2,080	197,836
15	3,330	39,550	17,649	18,860	79,389
16	158,070	25,650	3,761		187,481
17	14,575	42,420	8,678	1,950	67,623
18	10,185	14,535	6,003		30,723
19	1,820	64,360	1,668		67,848
20	0	0	1,071		1,071
21	87,400	8,480	6,848	8,320	111,048
22	0	116,755	294		117,049
23	1,870	0	306		2,176
24	0	370	421		791
25	0	0	855		855
26	0	2,500	1,416		3,916
27	660	0	322		992
28	1,730	0	9,078		10,808
29	0	0	5,011		5,011
30	0	0	5,509		5,509
Totals	660,630	366,440	174,719	76,010	1,277,799

loads were handled by a separate computation, and the dependency of the nitrogenous decay rate on temperature was expressed as

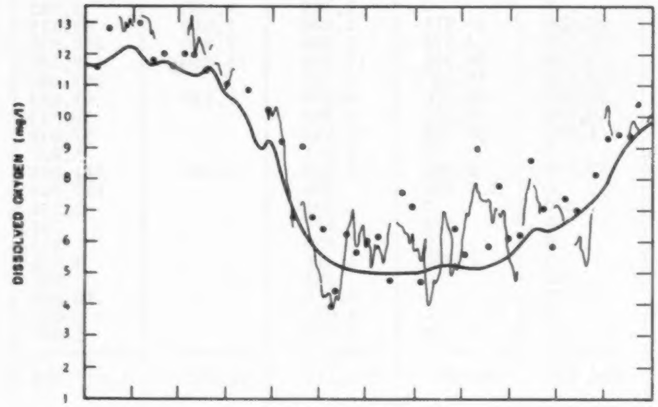
$$K_n = .00475 - .00184 + .000326\ T^2 - .0000170\ T^3 + .000000479\ T^4$$

Reaeration rates were calculated from the O'Connor-Dobbins (1958) formula (see Chapter III, Section 6.1.5). Dispersion coefficients were obtained from observations of salinity intrusion to Torresdale (Segment 7), and ranged from 4 square miles/day at Trenton (Segment 1) to 7 square miles/day at Liston Point (Segment 30). In Figure 7.32 is shown a comparison of measured and computed DO concentrations for a one year period at three segments in the Delaware (Pence et al. 1968).

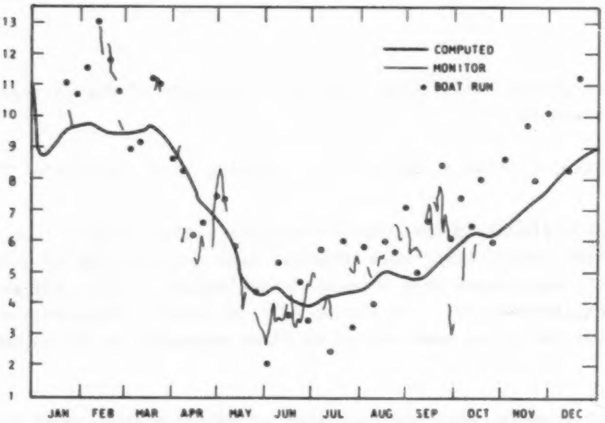
During the 1965 drought, when the intrusion of salinity threatened the water supply of many of the upstream municipalities, the DECS model was operated to predict salinity profiles



(a) BRISTOL-SECTION 4

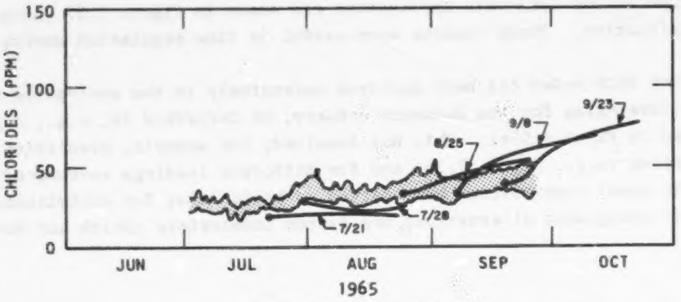


(b) TORRESDALE-SECTION 7

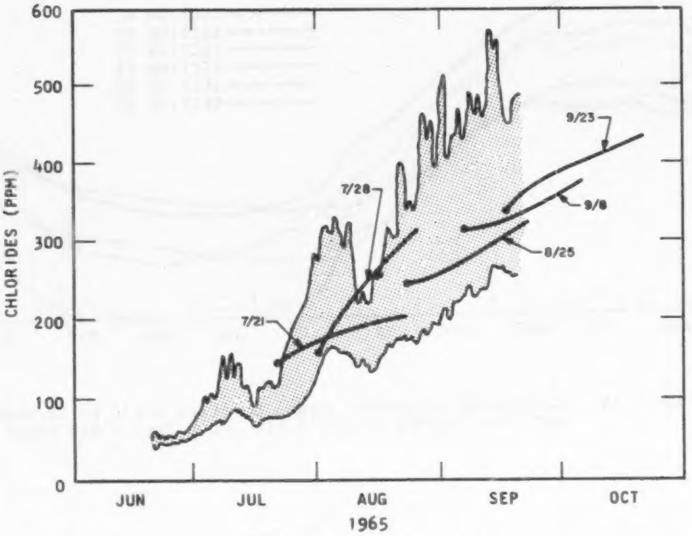


(c) DELAWARE MEMORIAL BRIDGE-SECTION 22

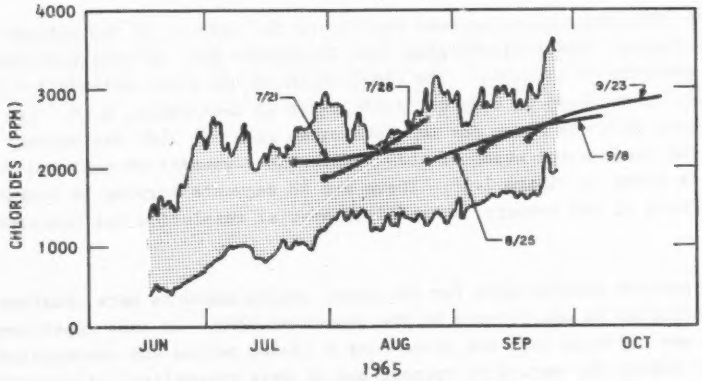
Fig. 7.32 Comparison of Observed DO and DECS Model Calculations for 1964 data.



TORRESDALE (SECTION 7)



FORT MIFFLIN (SECTION 15)



DELAWARE MEMORIAL BRIDGE (SECTION 22)

Fig. 7.33 Thirty-day forecasts of clorinity in Delaware estuary. From Jeglic and Pence (1968).

Example computations from this application are shown in Figure 7.33 along with the envelope of observed salinities. These results were useful in flow regulation during the drought.

The DECS model has been employed extensively in the evaluation of water quality management strategies for the Delaware estuary, as described in, e.g., Jeglic and Pence (1968) and reported in FWPCA (1966). This has involved, for example, prediction of DO profiles for various inflows (e.g., Figure 7.34) and for different loadings corresponding to treatment levels. The model computations have served as basic input for optimization calculations using a variety of management alternatives and system constraints (Smith and Morris 1969).

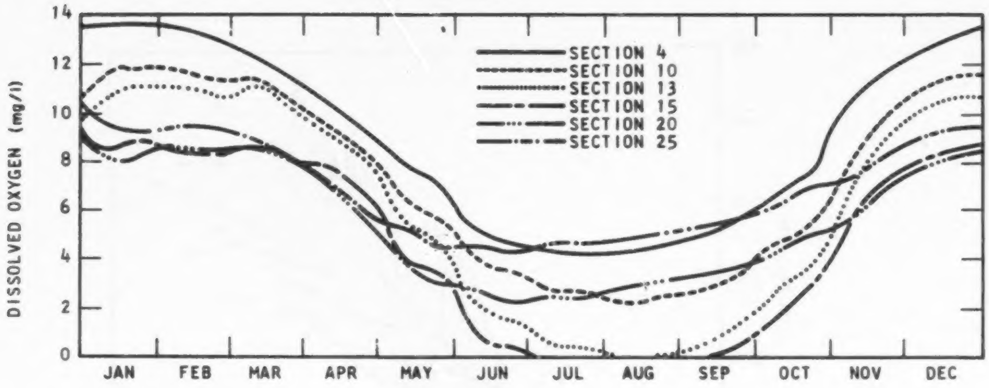


Fig. 7.34 Calculated dissolved oxygen profiles for 1 in 25 year flow and 1964 loading (Table 7.5). From Jeglic and Pence (1968).

3.2 THE POTOMAC ESTUARY

The DECS model has also been applied to the estuary of the Potomac (Figure 7.35), one of the principal rivers discharging into Chesapeake Bay, and which drains the metropolitan area of the District of Columbia. The tidal reach of the river extends 116 miles from Chesapeake Bay to the head of tide at Little Falls in Washington, D. C. The Potomac is an important source of fresh water for the Washington area; in 1967 the Potomac was supplying over 70% of the fresh water needs of this area. The segmentation employed in the modeling of the Potomac is shown in Figure 7.35. There are 28 segments varying in length from 2 miles in the upper portion of the estuary, where finer spatial resolution was required, to 6 miles near the mouth.

Dispersion coefficients for the first twelve segments were obtained from a dye diffusion study conducted in the Potomac in the summer of 1965. In this experiment 341 pounds of Rhodamine WT was injected into the river over a 13-day period and concentrations measured with a fluorometer during the period of release and 21 days thereafter. A segmented model (with slightly finer segmentation than that of Figure 7.35) solved on an analog computer was used

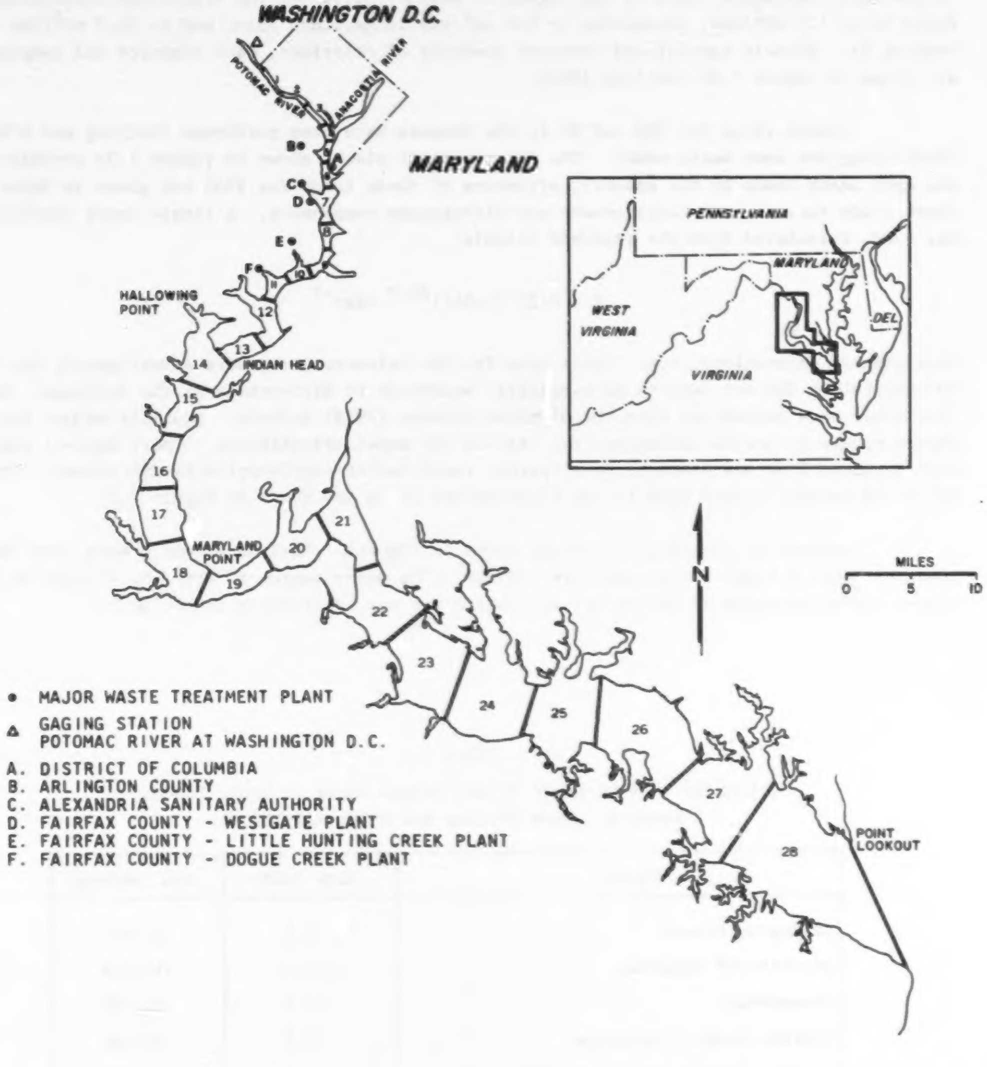

WASHINGTON D.C.
POTOMAC RIVER
ANACOSTIA RIVER
MARYLAND
PENNSYLVANIA
MARYLAND
DEL
WEST VIRGINIA
VIRGINIA
HALLOWING POINT
INDIAN HEAD
MARYLAND POINT
POINT LOOKOUT
N
MILES
0
5
10
A
B
C
D
E
F
12
13
14
15
16
17
18
19
20
21
22
23
24
25
26
27
28
● MAJOR WASTE TREATMENT PLANT
△ GAGING STATION POTOMAC RIVER AT WASHINGTON D.C.
A. DISTRICT OF COLUMBIA
B. ARLINGTON COUNTY
C. ALEXANDRIA SANITARY AUTHORITY
D. FAIRFAX COUNTY - WESTGATE PLANT
E. FAIRFAX COUNTY - LITTLE HUNTING CREEK PLANT
F. FAIRFAX COUNTY - DOGUE CREEK PLANT

Fig. 7.35 Potomac River showing model segmentation.

to determine the dispersion coefficients by a trial-and-error process. These coefficients ranged from .05 mi^2/day at Chain Bridge to 1.0 mi^2/day at Hallowing Point, the lower boundary of the study area. The remaining dispersion coefficients were determined from trial-and-error calculations of chlorine concentration using the segmented model of Figure 7.35. Thus at Indian Head, the upper limit of the region of saline intrusion, the dispersion coefficient was found to be 1.5 mi^2/day, increasing to 6.0 mi^2/day at Maryland Point and to 10.0 mi^2/day at Segment 22. Example spatial and temporal profiles of chlorides, both measured and computed, are shown in Figure 7.36 (Hetling 1968).

Computations for BOD and DO in the Potomac have been performed (Hetling and O'Connell 1968) using the same basic model. The six treatment plants shown in Figure 7.35 constitute the main waste loads to the estuary; estimates of these loads for 1966 are given in Table 7.6. These loads include both carbonaceous and nitrogenous components. A single decay coefficient was used, calculated from the standard formula

$$K = 0.23\ (1.047)^{20-T}\ (\text{day}^{-1})$$

More complex expressions, e.g., those used for the Delaware work, were investigated, but the DO calculation did not seem to be especially sensitive to differences in the formulae. Reaeration rates were calculated from the O'Connor-Dobbins (1958) formula. Explicit values for the oxygen uptake by bottom sediments were used in the model calculations. These benthal loads were obtained from measurements by a benthal respirometer supplemented by COD values. The values of benthal uptake used in the computations of DO are shown in Figure 7.37.

Example calculations of DO are shown in Figures 7.38-7.40 in which were used the loads of Table 7.6 and the appropriate inflows. The major source of error is thought to be the effects of photosynthesis in the estuary, which are not represented in the model.

TABLE 7.6

Estimated 1966 Ultimate Oxygen Demand Loads to Upper Potomac Estuary. From Hetling and O'Connell (1968).

Plant	Flow (MGD)	UOD (lb/day)
Arlington County	17.2	43,400
District of Columbia	232.9	318,000
Alexandria	14.1	11,700
Fairfax County: Westgate	9.2	18,400
Fairfax County: Little Hunting Creek	2.4	2,000
Fairfax County: Douge Creek	1.2	1,200

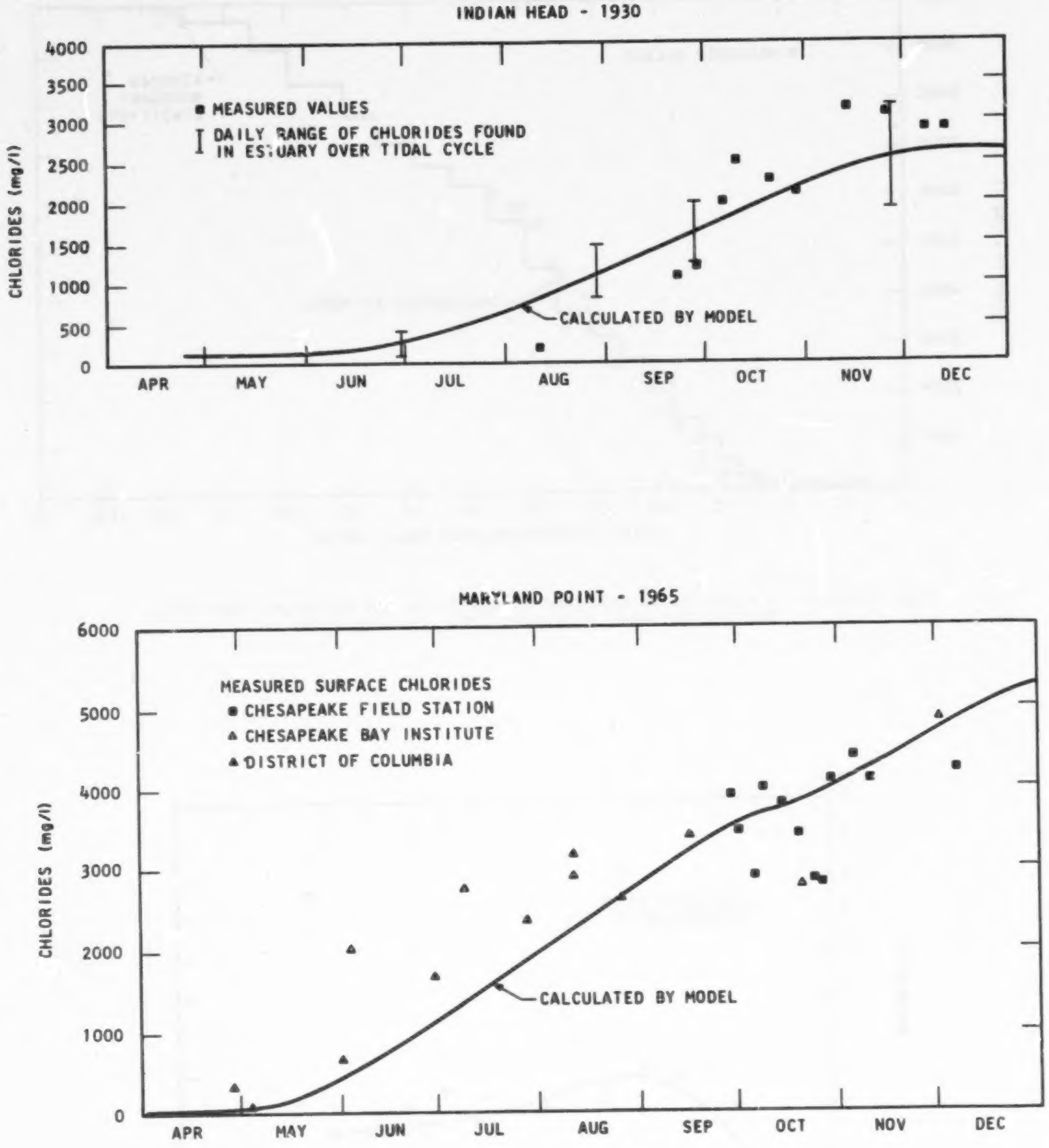


Fig. 7.36(a) Comparisons of measured chlorides and calculations using chloride model. From Hetling (1968).

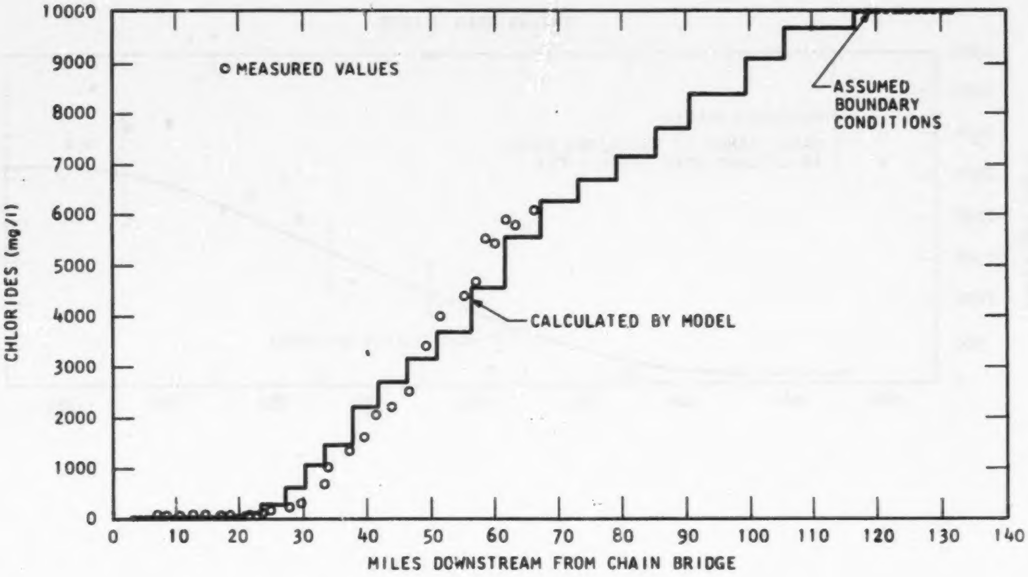


Fig. 7.36(b) Comparison of measured chlorinities and model calculations, Potomac Estuary, 8 October 1965 (Hetling 1968).

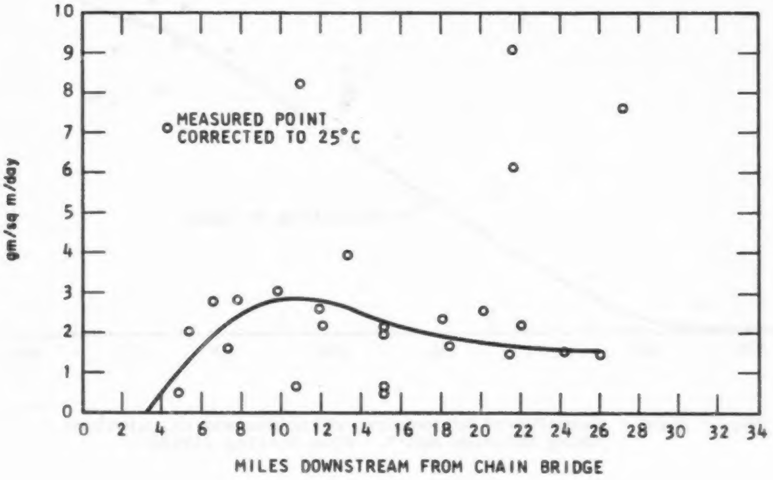


Fig. 7.37 Benthal uptake in Potomac Estuary (Hetling and O'Connell 1968).

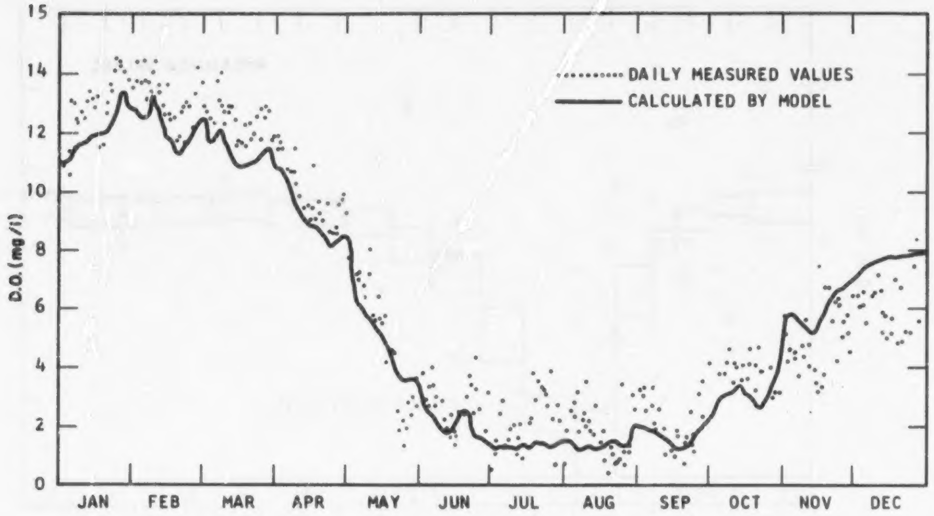


Fig. 7.38 Comparison of calculated and measured DO values for Potomac. From Hetling (1969).

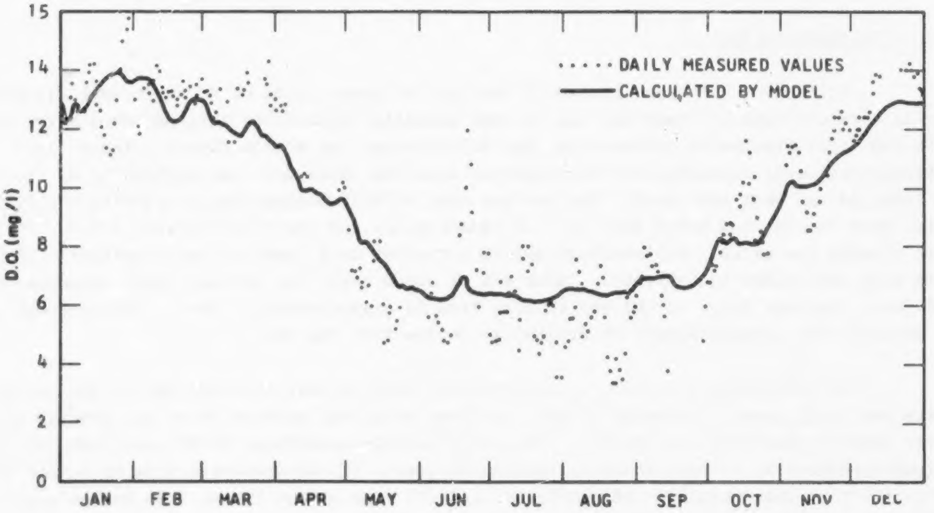


Fig. 7.39 Comparison of model calculations with 1965 DO data at Memorial Bridge, Segment 2, Potomac Estuary. Hetling (1969).

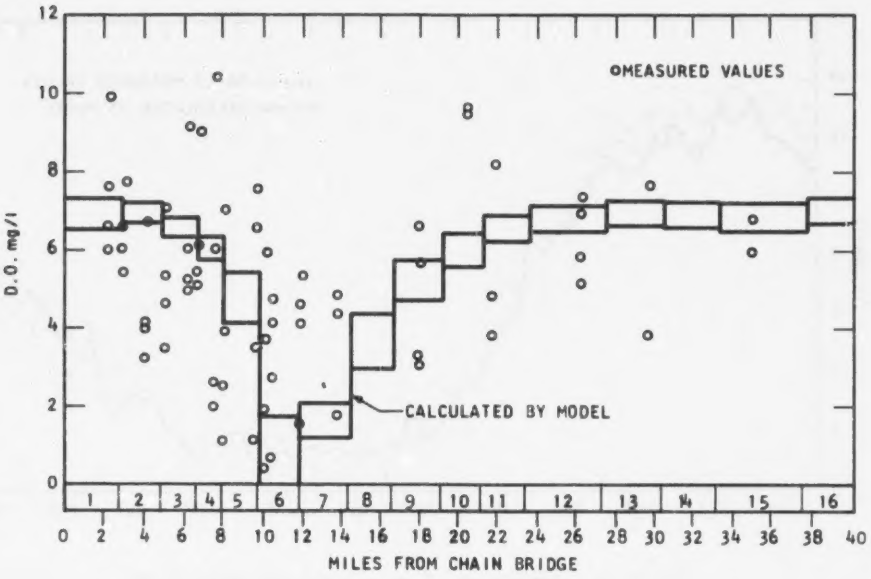


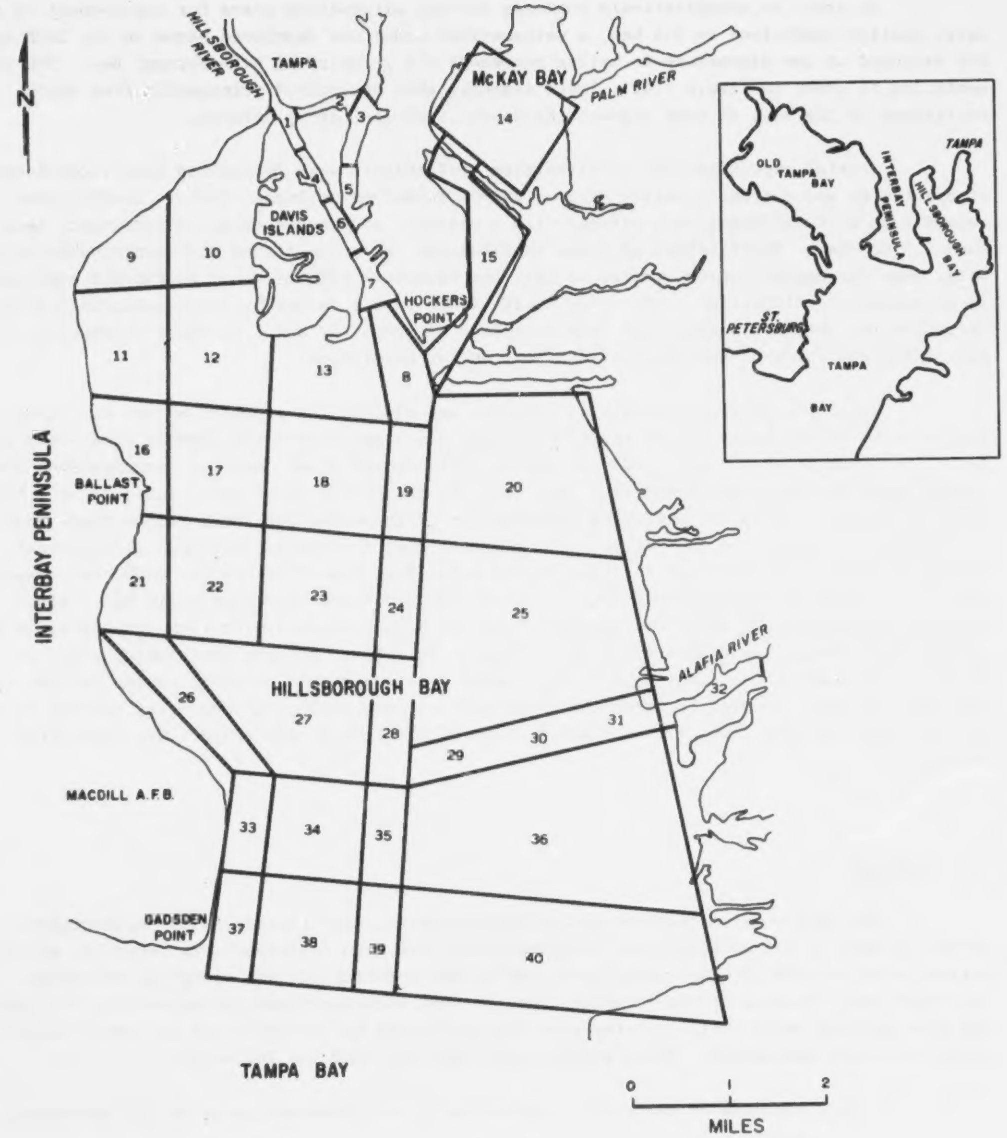
Fig. 7.40 Comparison of measured and computed DO, Potomac Estuary, 10 August to 1 September 1965 (Hetling and O'Connell 1968).

3.3 HILLSBOROUGH BAY

Hillsborough Bay is located on the Gulf of Mexico side of South Central Florida. The bay is a natural arm of Tampa Bay and is approximately eight miles long and four miles wide with two major freshwater tributaries, the Hillsborough and Alafia Rivers (Figure 7.41). The Interbay Peninsula separates Hillsborough Bay from Old Tampa Bay, and is bounded by the city of Tampa on the west and north. The surface area of Hillsborough Bay (including the harbor area, Port Sutton, and McKay Bay) is 39.6 square miles and the total volume is 8.3 x 10^9 cubic feet at mean low water. Hillsborough Bay is a typical Gulf Coast estuary, generally shallow with very weak tides and current. Tides are of mixed type, the diurnal tidal range being 2.8 feet. Average depth of the bay at mean tide is approximately 9 feet. Hillsborough River is normally the largest source of freshwater inflow into the Bay.

In 1965 FWPCA undertook a water quality study of Hillsborough Bay at the request of state and local agencies because of odor problems along the western shore and general poor water quality conditions of the bay. The water quality conditions in Hillsborough Bay had degraded because of a combination of various factors: (1) inadequately treated sewage effluents, (2) high concentrations of nutrients, and (3) high oxygen demand from bottom sediment deposits. All these factors contributed to excessive algae growth and poor water quality conditions in certain areas of the bay.

One of the conclusions of this study (FWQA 1969) was that the obnoxious odors along the western shore of Hillsborough Bay were the result of the death and decay of the marine algae Gracilaria which constitutes 98% of the attached algal crop in Hillsborough Bay (in contrast to 2% in nearby Tampa Bay). Death of Gracilaria was found to be precipitated by


N
TAMPA
HILLSBOROUGH RIVER
McKAY BAY
PALM RIVER
DAVIS ISLANDS
HOCKERS POINT
BALLAST POINT
INTERBAY PENINSULA
HILLSBOROUGH BAY
ALAFIA RIVER
MACDILL A.F.B.
GADSDEN POINT
TAMPA BAY
1
2
3
4
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35
36
37
38
39
40
0
1
2
MILES
OLD TAMPA BAY
INTERBAY PENINSULA
HILLSBOROUGH BAY
TAMPA
ST. PETERSBURG
TAMPA BAY

Fig. 7.41 Hillsborough Bay model segmentation.

high freshwater inflows (i.e., in excess of 2,400 cfs) which lowered the chlorinity below 6 ppt, the salinity stress point for Gracilaria. When the freshwater inflow exceeded 2,400 cfs, the Gracilaria standing crop was substantially reduced, oxygen was depleted, and sulfides were produced.

In order to quantitatively evaluate various alternative plans for improvement of the water quality conditions in the bay, a mathematical model was developed based on the DECS model but extended to two dimensions to better represent the geometry of Hillsborough Bay. The segmentation is shown in Figure 7.41. These segments were determined principally from depth variations in the bay; in each segment the depth is approximately uniform.

Initial approximations of dispersion coefficients were determined from a consideration of dye tracer and current velocity data using the relations in Bunce (1967). Coefficients ranged from 0.70 mi^2/day to 6.0 mi^2/day with a majority of the dispersion coefficients less than 2.0 mi^2/day. Verification of these coefficients was accomplished with winter chlorinity data, when freshwater inflow was low so that the advective effects could be assumed negligible in comparison to dispersion. Advective coefficients were obtained by reproducing chlorinity distributions obtained during high flow periods. Figures 7.42 and 7.43 shows comparisons of calculated and observed chlorinities for both inflow conditions.

Using the developed model, an analysis was made of the proposal by the U.S. Corps of Engineers to divert water out of the Hillsborough River Basin into the Sixmile Creek-Palm River Basin. Maximum diversion was 1,200 cfs out of Hillsborough River, and the corresponding discharge from Palm River was 2,000 cfs. The flow for the Alafia River was assumed to be 1,500 cfs. Shown in Figure 7.44 is the predicted distribution of chlorides for these inflow conditions. Comparison of Figure 7.44 and Figure 7.43 indicates that for the Hillsborough flow approximately the same, a significant increase in the Palm River flow (169 cfs to 2,000 cfs) results only in a slight decrease of chlorides along the western shore of Hillsborough Bay. Since chloride concentrations along the western shore are highly sensitive to flow variations in the Hillsborough River, the diversion of the inflow to Palm River appears preferable, since it would result under these conditions in only minor fluctuations in chloride concentrations in the critical area. Therefore, from the standpoint of odor production and water quality in Hillsborough Bay, the flow diversion alternative of the Four Rivers Project was considered desirable.

3.4 SUMMARY

The DECS model is perhaps not as sophisticated, particularly in its hydrodynamic terms, as many of the computational programs which have been developed more recently, and its coarse space and time scales render inaccessible the modeling of many estuarine phenomena. On the other hand, because of its relative computational efficiency and its capability for modeling the more salient water quality parameters, the DECS model has proved to be extremely useful in water pollution management. These applications have included the following:

(i) Analysis of the factors affecting DO and the sensitivity of the estuary to each;

(ii) Evaluation of alternatives such as relocation of outfalls, inflow augmentation, and levels of waste treatment to determine their efficacy in improving estuarine DO;

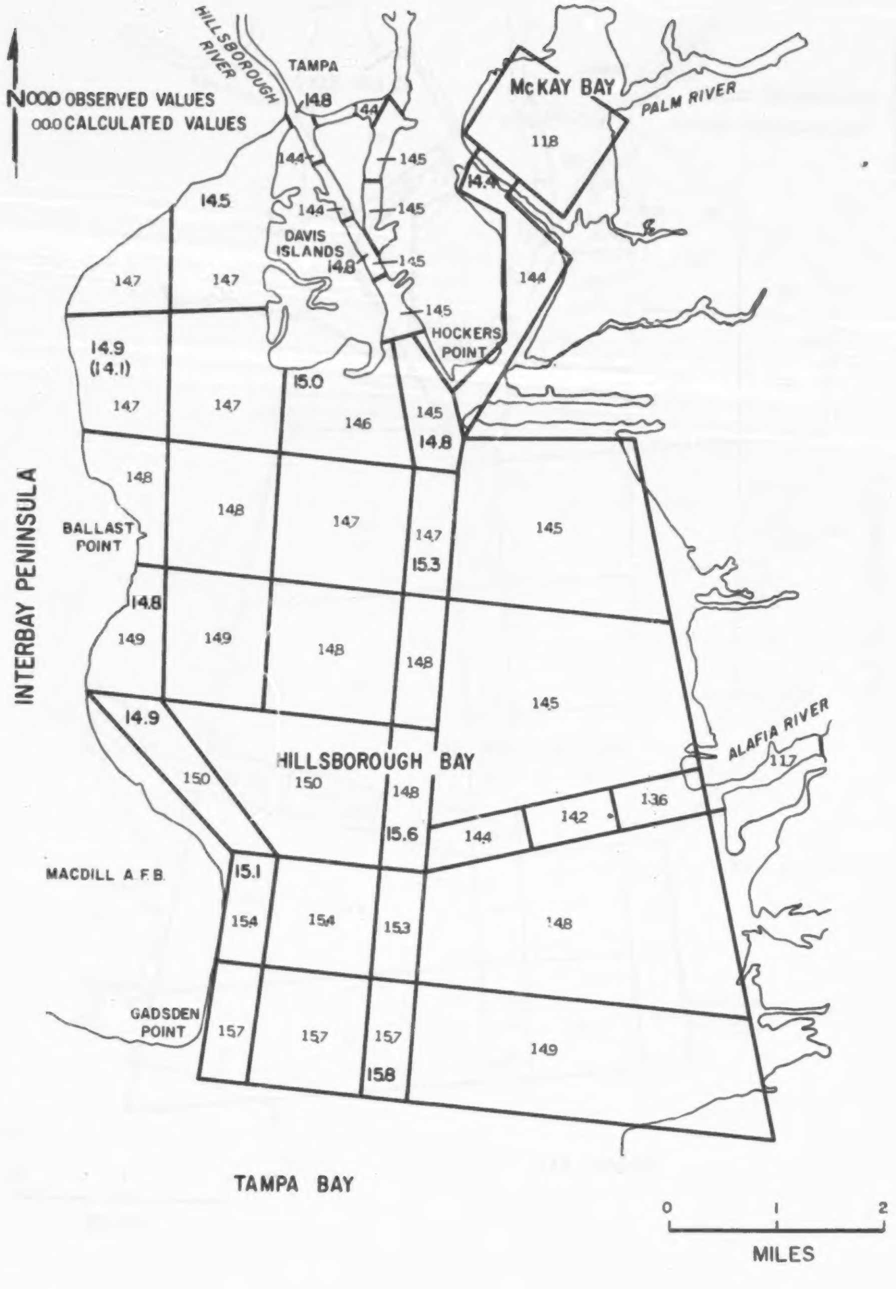
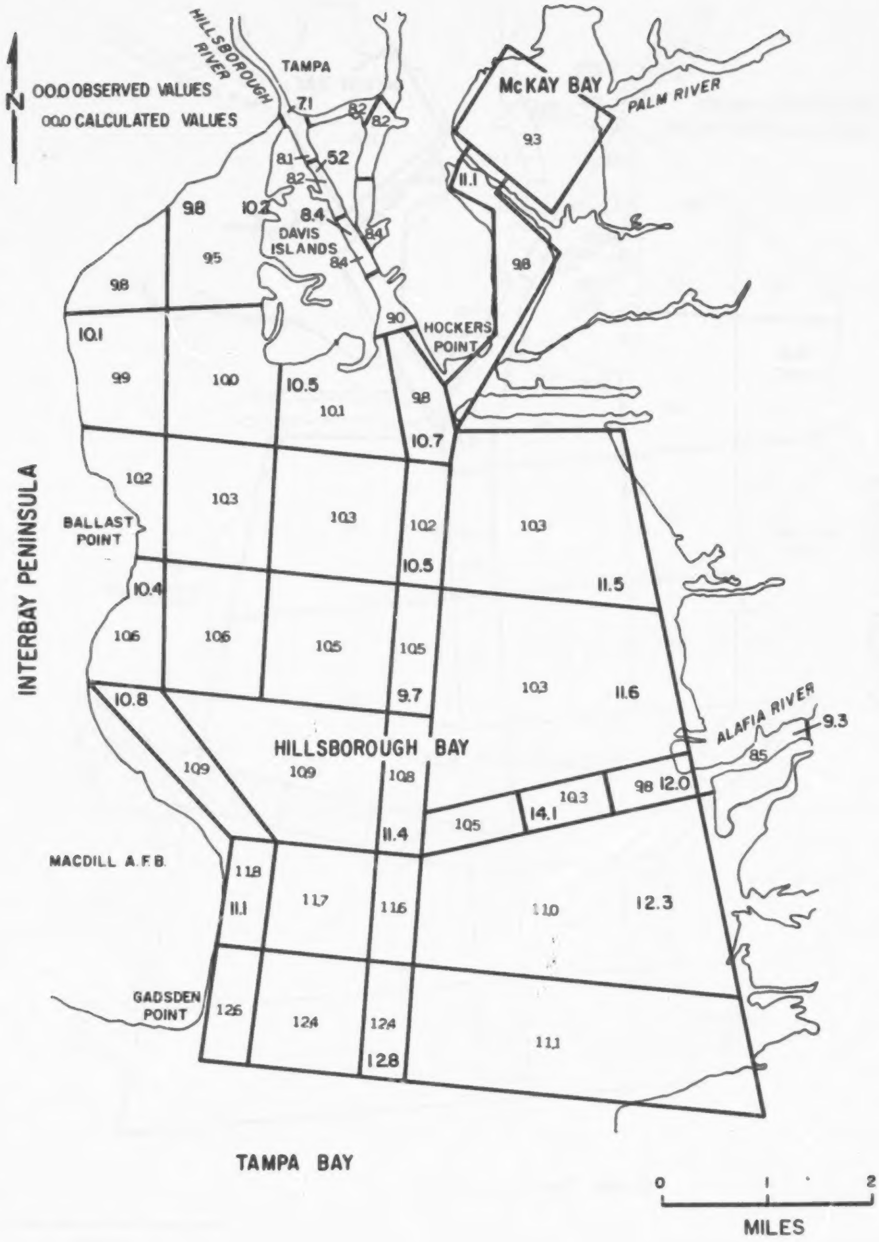

N
000 OBSERVED VALUES
000 CALCULATED VALUES
HILLSBOROUGH RIVER
TAMPA
McKAY BAY
PALM RIVER
DAVIS ISLANDS
HOCKERS POINT
INTERBAY PENINSULA
BALLAST POINT
HILLSBOROUGH BAY
ALAFIA RIVER
MACDILL A.F.B.
GADSDEN POINT
TAMPA BAY
14.8
14.4
14.5
14.7
14.9
(14.1)
15.0
14.6
11.8
15.3
14.9
15.0
15.6
15.1
15.4
15.7
15.8
14.2
13.6
11.7
0
1
2
MILES

Fig. 7.42 Observed and calculated chloride concentrations (ppt) December, January, February, and March, 1967-68.


N
00.0 OBSERVED VALUES
00.0 CALCULATED VALUES
HILLSBOROUGH RIVER
TAMPA
McKAY BAY
PALM RIVER
7.1
8.2
8.2
9.3
8.1
5.2
8.2
11.1
9.8
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8.4
DAVIS ISLANDS
8.4
8.4
9.5
9.8
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9.0
HOCKERS POINT
10.1
9.9
10.0
10.5
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10.7
INTERBAY PENINSULA
10.2
10.3
10.3
10.2
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BALLAST POINT
10.5
10.4
11.5
10.6
10.6
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10.5
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9.7
10.8
ALAFIA RIVER
9.3
HILLSBOROUGH BAY
8.5
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10.9
10.8
10.3
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12.0
14.1
10.5
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MACDILL A.F.B.
11.8
11.1
11.7
11.6
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12.3
GADSDEN POINT
12.6
12.4
12.4
12.8
11.1
TAMPA BAY
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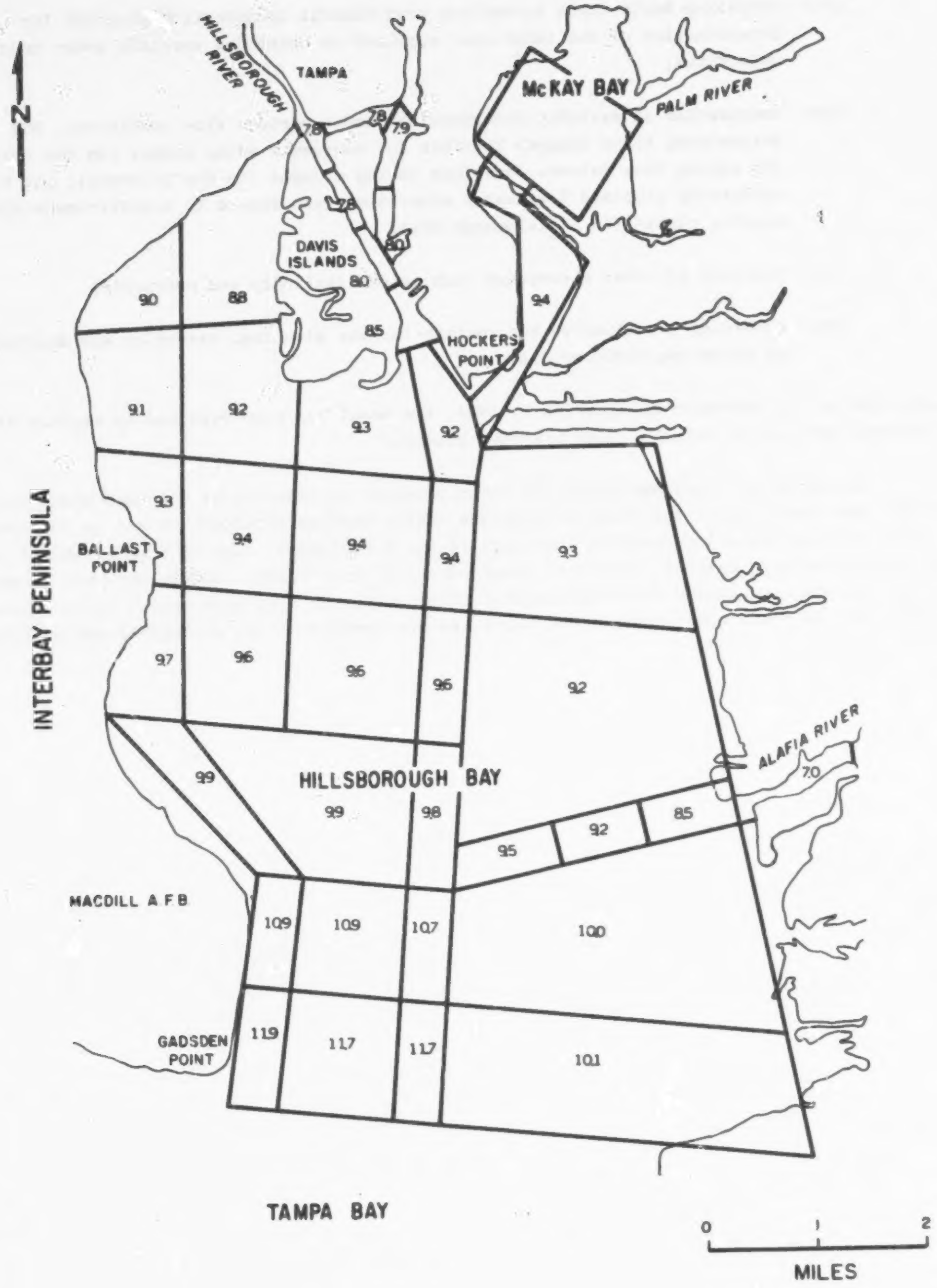
1
2
MILES

Fig. 7.43 Observed and calculated chloride concentrations (ppt) August, September, and October, 1967.



N
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DAVIS ISLANDS
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HOCKERS POINT
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INTERBAY PENINSULA
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BALLAST POINT
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ALAFIA RIVER
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HILLSBOROUGH BAY
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MACDILL A.F.B.
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GADSDEN POINT
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10.1
TAMPA BAY
0
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2
MILES

Fig. 7.44 Predicted effect of proposed flow diversion on chloride concentrations.

(iii) Providing basic input to various cost-benefit optimization programs for determination of the least-cost approach to obtaining specific water quality objectives;

(iv) Computation of salinity distributions under various flow conditions, for determining those reaches feasible for emergency water supply (in the Potomac), for aiding flow release decisions during drought (in the Delaware), and for evaluating proposed freshwater diversions with regard to salinity-sensitive aquatic plants (in Hillsborough Bay);

(v) Modeling of other parameters such as pH-alkalinity and nutrients;

(vi) Providing quantitative information for the planning, execution and analysis of estuarine field studies.

In addition to its extensive application by FWQA, the model has been employed by various state and federal agencies in water quality planning studies.

Certainly an important factor to the widespread application of the DECS model is the excellent documentation of the computer programs, which enables personnel to set up and operate the model without requiring detailed knowledge of its formulation. The DECS model should serve as a paradigm in this respect; continued development of water quality models not only is dependent upon advances in theory and computational techniques, but also upon making these advances available to the practicing engineer and water resource manager in an accessible and utilitarian form.

4. SAN FRANCISCO BAY

The San Francisco Bay and its associated systems (i.e., San Pablo Bay, Suisun Bay, and the Sacramento-San Joaquin Delta) comprise one of the major harbor and estuarine systems of the continental United States. Over sixty cities are situated on its periphery, presently discharging an estimated 660 million gallons per day of municipal-industrial wastewater. Demands are increasing on the freshwater inflows into the system, from municipal consumption, export to other areas of the state, and agricultural use in the Central Valley and Delta area. Salinity intrusion into the Delta during periods of low freshwater inflow has been a major problem to the farmlands and industries of the region.

The San Francisco Bay system, the Delta system and the Central Valley River system have been the subject of many modeling investigations, addressing their hydrology, hydrodynamics, salinity distribution, and quality indicators, and the methods employed encompass all of the techniques discussed previously. Of this profusion of studies, two estuarine models of particular interest are selected for discussion, the physical model of the U.S. Corps of Engineers (1963) and the numerical hydrodynamic-water quality model of FWQA developed under contract by Water Resources Engineers, Inc., (1968) (see also Feigner and Harris 1970, Orlob et al. 1967, Kaiser Engineers 1969).

4.1 CHARACTERISTICS OF THE BAY-DELTA SYSTEM

4.1.1 Physiographic and Hydrographic Features

San Francisco Bay per se is an irregular, elongated bay of some 50 miles length nearly landlocked with its only connection with the ocean at the Golden Gate (Figure 7.45). At its northern tip San Francisco Bay joins San Pablo Bay, and from this juncture the system extends eastward through Suisun Bay to the confluence of the Sacramento and San Joaquin Rivers and the sprawling Delta. The Sacramento and San Joaquin are the major sources of inflow to the Bay system. A number of smaller streams discharge into the Bay, but their combined annual flows are (nominally) less than 3% of the inflow from the Delta.

San Francisco Bay is generally quite shallow, averaging 20 feet in depth. The deepest region of the Bay is the Golden Gate where the depth is 382 feet at mean sea level. In contradistinction, however, about 50% of the total Bay area is less than 10 feet deep and about 68% is less than 20 feet deep. Due to this general shallowness, waves and currents cause considerable resuspension of sediment which results in highly turbid water, even during periods when little turbidity is being brought in by the major rivers. The southern part of San Francisco Bay below Dumbarton Bridge is characterized by extensive tidal flats and meandering sloughs. The total area of these tidal flats exposed at mean lower low water is some 57% of the high tide area (10,700 acres) of the Bay south of the Bridge. The total area of the sloughs is about 22% of the total tidal area.

The upper bays, San Pablo and Suisun, are shallower than San Francisco Bay. Suisun Bay, like South San Francisco Bay, is a shallow body of water with meandering tidal channels

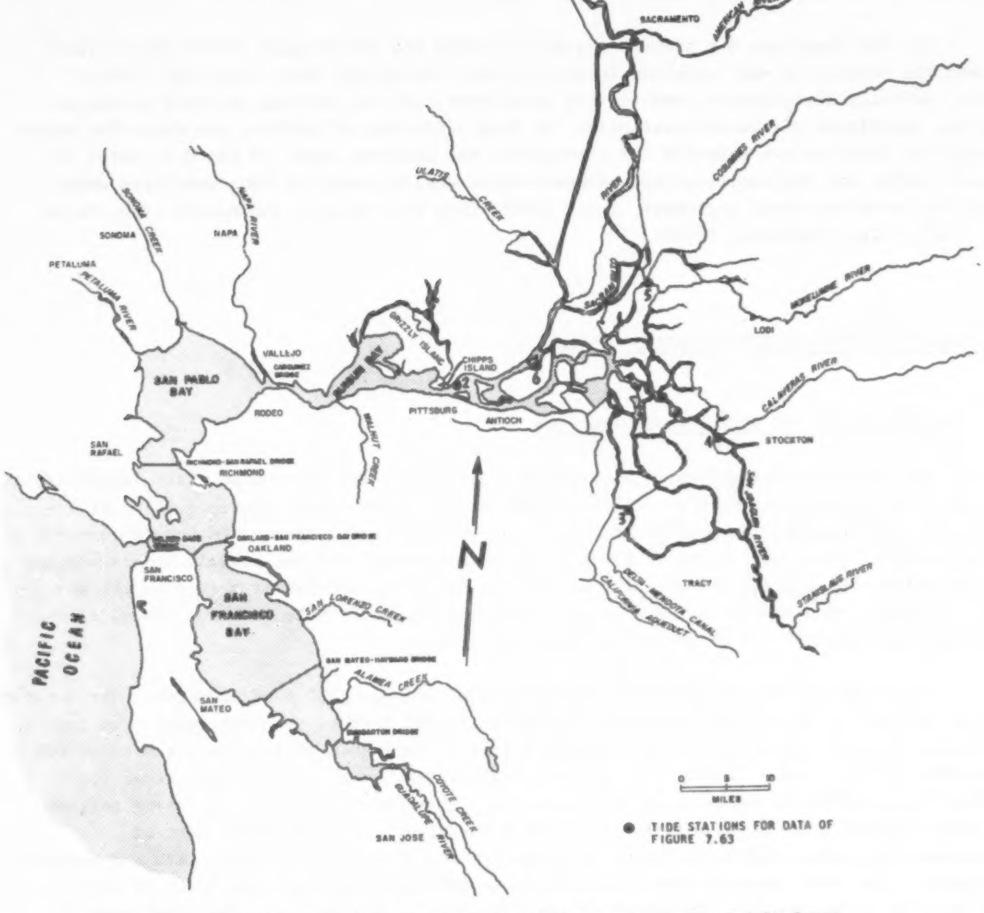

SACRAMENTO
AMERICAN RIVER
COSUMNES RIVER
ULATIS CREEK
SACRAMENTO RIVER
MOKELUMNE RIVER
LODI
SONOMA CREEK
NAPA RIVER
SONOMA
NAPA
PETALUMA
PETALUMA RIVER
GRIZZLY ISLAND
CHIPPS ISLAND
VALLEJO
CARQUINEZ BRIDGE
SAN PABLO BAY
RODEO
WALNUT CREEK
PITTSBURG
ANTIOCH
CALAVERAS RIVER
STOCKTON
SAN RAFAEL
RICHMOND-SAN RAFAEL BRIDGE
RICHMOND
OAKLAND-SAN FRANCISCO BAY BRIDGE
OAKLAND
SAN FRANCISCO
SAN FRANCISCO BAY
SAN LORENZO CREEK
PACIFIC OCEAN
N
SAN JOAQUIN RIVER
DELTA-MENDOTA CANAL
CALIFORNIA AQUEDUCT
TRACY
STANISLAUS RIVER
SAN MATEO-HAYWARD BRIDGE
ALAMEA CREEK
SAN MATEO
DUMBARTON BRIDGE
COYOTE CREEK
GUADALUPE RIVER
SAN JOSE
1
2
3
4
5
6
0 5 10
MILES
● TIDE STATIONS FOR DATA OF FIGURE 7.63

Fig. 7.45 Location map, San Francisco Bay and Sacramento - San Joaquin Delta System.

and extensive tidal flats, and is almost completely surrounded by salt marshes. These marshes are traversed by a system of tidal sloughs which overflow at higher tide to flood the marshes. Carquinez Strait, the waterway joining San Pablo and Suisun Bays, varies in width from 2,700 feet to 6,900 feet and has depths ranging from 40 to 80 feet on the western end, 108 feet in the central portion, and 67 feet on the eastern end.

Tides in San Francisco Bay are of the mixed type and have a mean range (i.e., mean high to mean low) of 3.99 feet with a mean great diurnal range of 5.72 feet. The greatest mean tidal range is in the southern part of the Bay. The mean range in South Bay is about 6 feet and at Alviso the mean range reaches 7.22 feet. The range on the western shore is slightly more than that on the eastern shore of South Bay due to the Coriolis effect. The mean ranges in San Pablo Bay and Carquinez Strait are 4.45 feet and 4.40 feet. Suisun is evidently more subject to wind tides and the variations of inflow, and seems to average 4.0 feet. Influence of the tide is observed far inland and during low flow can extend well over a hundred miles from the Golden Gate. For example, during low flow, the mean tidal range at Sacramento, 110 miles from the Golden Gate, is 2.5 feet.

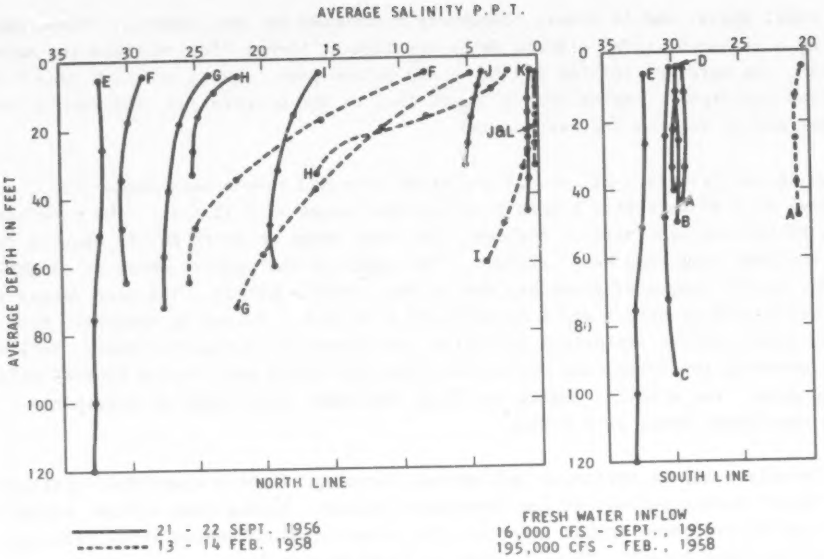
San Francisco Bay is typically well-mixed, becoming slightly stratified upstream from the Carquinez Strait during periods of low freshwater inflow. During high inflow, slight stratification may be evidenced in San Francisco Bay proper and pronounced stratification obtained in the Carquinez Strait. This is exemplified by Figure 7.46.

The Delta is an area of approximately 1,100 square miles of highly developed, irrigated land lying between Sacramento on the north and Tracy on the south, and extending westward from Stockton to the confluence of the Sacramento and San Joaquin Rivers near Collinsville. The Delta was at one time an extensive marshy area and possesses very fertile peat soils. During the last century practically the entire region has been drained and reclaimed into more than 50 islands now used principally for agriculture. Nearly all of the islands lie below sea level, some over 18 feet.

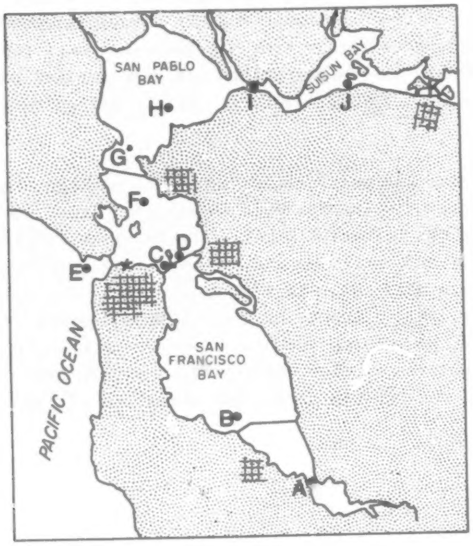
A number of rivers enter the Delta region along its eastern boundary. The major streams are, of course, the Sacramento and San Joaquin Rivers; others include the Cosumnes River, the Mokelumne River, and the Calaveras River. The Delta is interlaced by more than 700 miles of meandering channels and waterways which have a total surface area of more than 75 square miles and a volume more than twice that of Suisun Bay. The varying inflows to the Delta from the tributary rivers, the influence of tides in the western Delta, the consumption of water within the region, and the varying amounts of water exported from the Delta all contribute to extremely complex patterns of flow within the area. In many of the smaller channels, and even in some reaches of the San Joaquin River, the direction of flow may be reversed at certain times of the year.

4.1.2 Water Quality

The principal types of discharge in the Bay system are municipal and industrial effluents and agricultural drainage. An appreciation of the volumes involved can be gained from Table 7.7. Water quality zones are delineated in Figure 7.47. DO levels throughout most of San Francisco Bay proper are high, consistently above 80% saturation. There is a significant DO depletion problem in the region below Dumbarton Bridge, which has been studied using a steady-state finite section model (Consoer, Townsend and Associates 1968). A problem throughout the Bay is toxicants associated with wastewater discharges. Increasingly in recent



(a) OBSERVED SALINITIES


SAN PABLO BAY
SUISUN BAY
H
I
J
G
F
C
D
E
PACIFIC OCEAN
SAN FRANCISCO BAY
B
A

(b) STATION LOCATIONS

Fig. 7.46 Average salinities in San Francisco Bay.

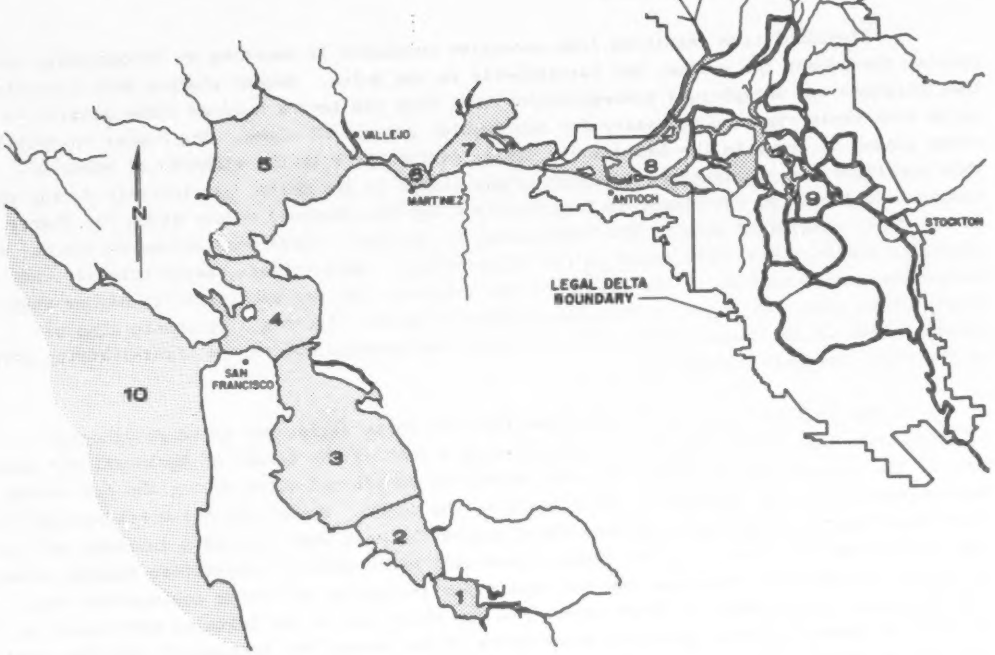

VALLEJO
5
7
6
MARTINEZ
8
ANTIOCH
9
STOCKTON
N
LEGAL DELTA BOUNDARY
4
SAN FRANCISCO
10
3
2
1

Fig. 7.47 San Francisco Bay-Delta area showing water quality zones.

Water Quality Zone (Fig. 7.47)	Waste Source	Flow (MGD)	BOD (10^6 Lb/Yr)	Total Nitrogen (10^6 Lb/Yr)
1, 2 & 3	Municipal	273	384	95
	Discrete Ind.	4	-	-
	S. Bay Total	277	384	95
4	Municipal	78	90	22
	Discrete Ind.	1	-	-
	Cent. Bay Total	79	90	22
5, 6 & 7	Municipal	55	52	13
	Discrete Ind.	18	65	23
	N. Bay Total	73	117	36
8 & 9	Municipal	120	120	29
	Discrete Ind.	36	21	-
	Delta Total	156	141	29
TOTAL: Mun. and Ind.		585	732	182

TABLE 7.7

Annual (1965) Average Characteristics of
Untreated Municipal and Industrial Wastewaters.
From Program Staff (1969)

years, low DO concentrations have been observed locally in parts of the Delta. The two principal contributing factors to this condition are the BOD from municipal and industrial wastes, and excessive algal growths.

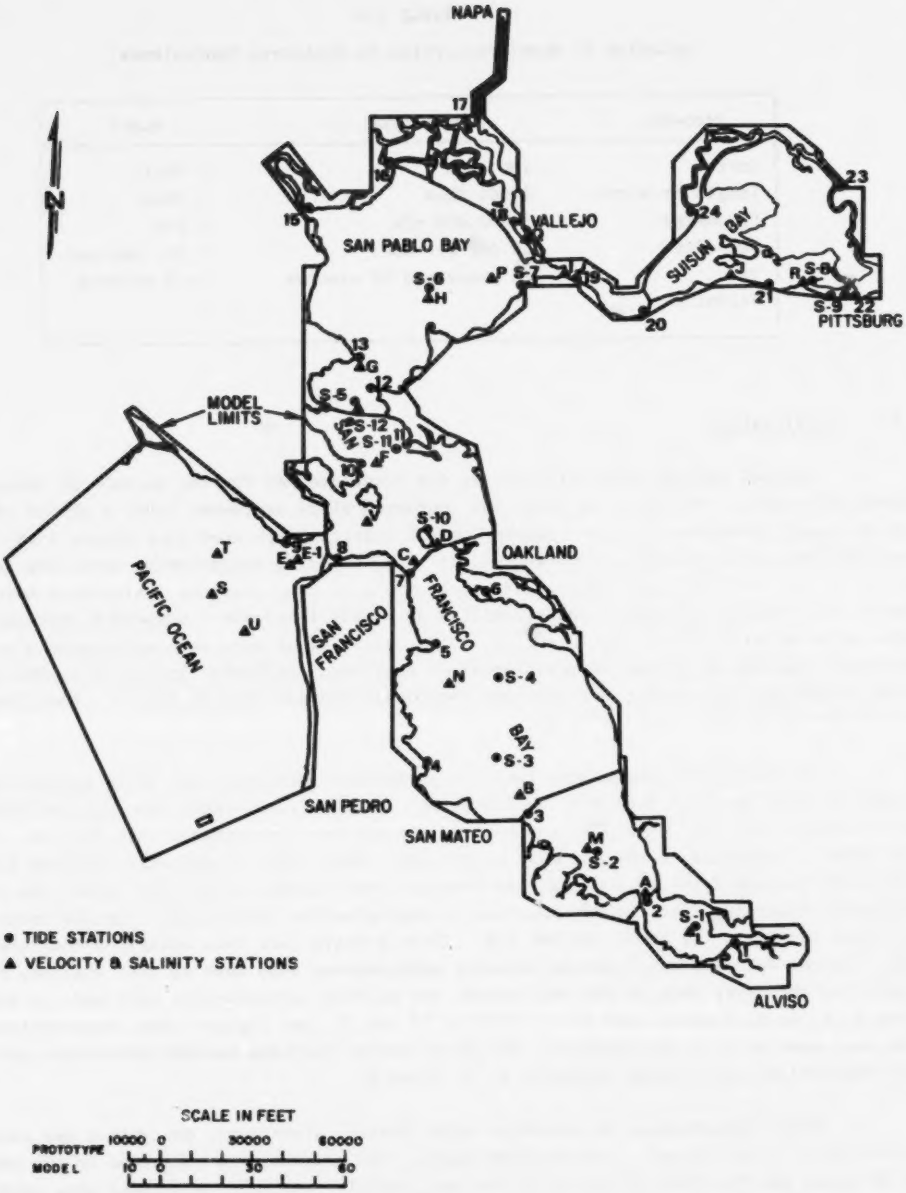
Biostimulation resulting from excessive nutrients is becoming an increasingly serious problem throughout the system, but particularly in the Delta. Recent studies have indicated that nitrogen and phosphorous concentrations were from ten to one hundred times greater in the Delta than those reported necessary for substantial growths of algae. The higher concentrations tended to occur in the San Joaquin River, particularly in the vicinity of Stockton. This condition has precipitated extensive algae blooms in the Delta, particularly during the summer. Evidences of enrichment in San Francisco Bay are observed mainly along the shores and in the tidal reaches of some of the tributaries to the Bay. Algal populations in the Bay are generally smaller than those found in the Delta system. Nevertheless, total nitrogen and phosphorus concentrations in the waters of San Francisco Bay are substantially higher than the levels where either nitrogen or phosphorus might be growth-limiting. It should also be remarked that in San Francisco Bay there is algal suppression due to the light-limiting effects of the high inorganic turbidity.

The problem of salinity intrusion into the Delta region was noted previously. Salinity intrusion is now partially controlled as a part of the Bureau of Reclamation's operation of its Central Valley Project by the release of additional water during the dry season from reservoirs in the Sacramento River Basin to the north. These controlled releases of stored water have largely eliminated the very low flows of the past when chlorides intruded well up into the Sacramento River. In the future there will be increasing competition between demands for water for salinity repulsion and for export for irrigation and other consumptive uses. With increased withdrawals of fresh water from the south end of the Delta as more water is exported to water-deficient areas in other parts of the State, the problem of salinity intrusion can be expected to be seriously aggravated. The object of many barrier plans has been to isolate fresh water from salt water, and thereby conserve water now required for salinity repulsion.

4.2 THE PHYSICAL MODEL

The San Francisco Bay estuary model developed and constructed by the U. S. Corps of Engineers (1963) is a physical hydraulic model which represents all of San Francisco Bay, Suisun Bay, the lower reach of the Delta to the confluence of the Sacramento and San Joaquin River, and 17 square miles of the Pacific Ocean beyond the Golden Gate (Figure 7.48). The model is located in Sausalito, California, and covers an area of approximately an acre. The vertical-to-horizontal scale distortion is 10:1 and the time scale is 1:100. Specific data on the model-prototype scale relations are given in Table 7.8.

The effect of the tides is simulated by means of a primary tide generator located at the seaward end of the model and a secondary tide generator located at the upstream limit of the model at the head of Suisun Bay. This secondary unit is synchronized with the primary in order to reproduce proper ebb and flood flows at the upper limit of the model. Salinity is regulated to the exact concentration required by mixing salt water and tap water in the sump. Freshwater inflow points are located around the model to simulate stream flow. The model has been applied extensively to studies of shoaling in the Bay, and to evaluation of the effects of proposed barriers on the Bay system.


NAPA
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SUISUN BAY
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PITTSBURG
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G
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MODEL LIMITS
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OAKLAND
T
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U
PACIFIC OCEAN
SAN FRANCISCO
FRANCISCO
6
5
N
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BAY
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B
SAN PEDRO
3
SAN MATEO
M
S-2
A
2
S-1
L
ALVISO
● TIDE STATIONS
▲ VELOCITY & SALINITY STATIONS
SCALE IN FEET
PROTOTYPE 10000 0 30000 60000
MODEL 10 0 30 60

Fig. 7.48 San Francisco Bay physical model.

TABLE 7.8

Relation of Model Properties to Prototype Equivalents

Property	Prototype	Model
Depth	100 feet	1 foot
Length or Width	1,000 feet	1 foot
Discharge	1,000,000 cfs	1 cfs
Velocity	10 ft. per sec.	1 ft. per sec.
Time	24 hours and 50 minutes	14.9 minutes
Salinity	1	1

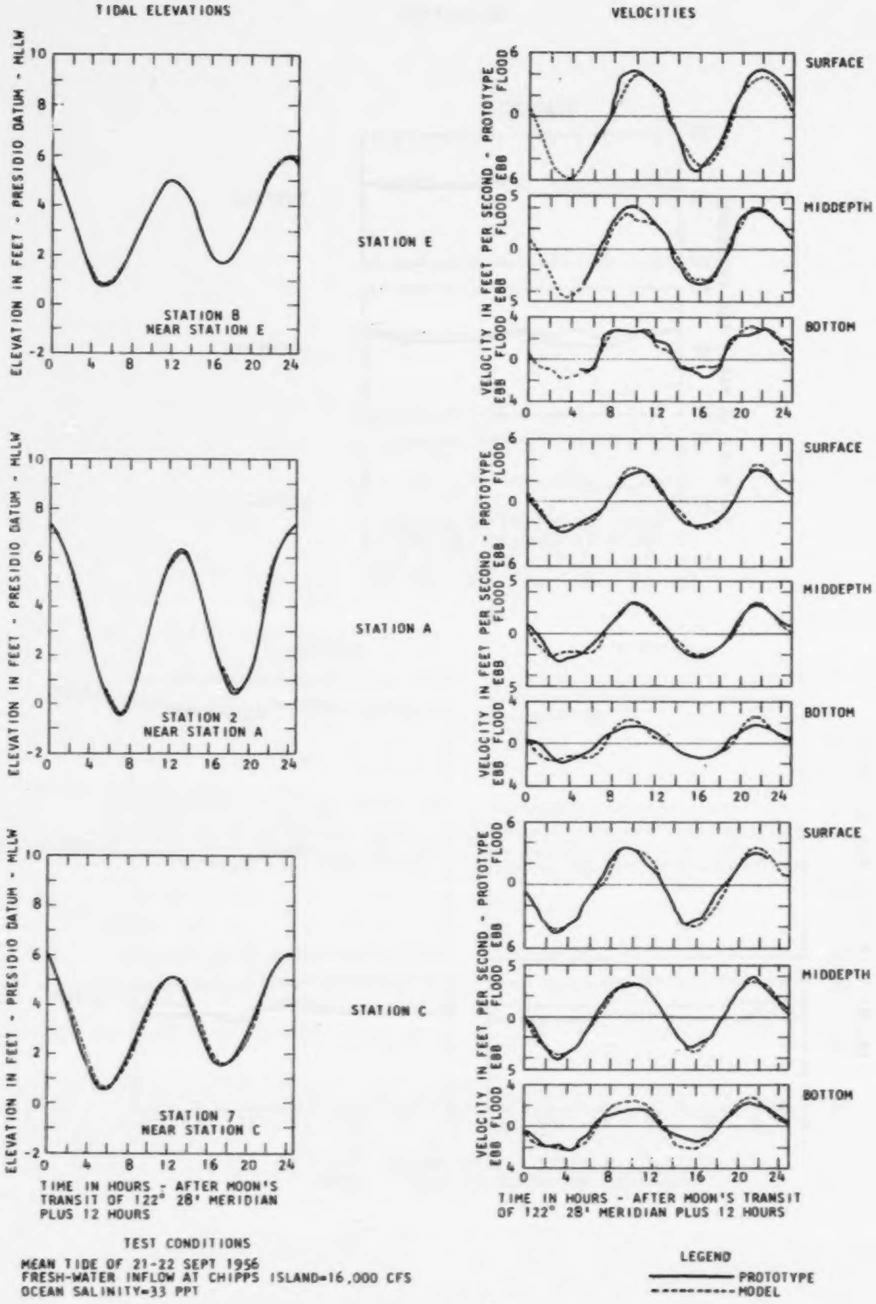
4.2.1 Verification

Several surveys were performed in San Francisco Bay for the purpose of obtaining verification data. The first of these was conducted 21-22 September 1956, a period of low, fairly steady freshwater inflow. Eleven control stations were used (see Figure 7.48) located over the deep-water channels. Current velocity and salinity measurements were made at 6 or 7 points in the vertical simultaneously at each of the 11 boat stations, velocities being measured at half-hourly intervals, and salinities at hourly intervals. Suspended sediment samples were collected at 6 of the boat stations. Tide observations were made concurrently at 24 shore stations. During the period of measurement, a sustained freshwater inflow of 16,000 cfs was being discharged into Suisun Bay from the Sacramento and San Joaquin Rivers. Flow from the other tributaries was practically nil.

To obtain data representative of high inflow conditions, two field surveys were conducted in 1958, on 13-14 February and 3-4 March. On the former date, the combined discharge of the Sacramento and San Joaquin Rivers into Suisun Bay was approximately 180,000 cfs. Discharges from other tributaries to the Bay were as follows: Napa River, 5,000 cfs; Petaluma River, 5,000 cfs; Alameda Creek, 3,500 cfs; and Mountain View Slough, 1,500 cfs. Thus, the total freshwater discharge into the Bay amounted to approximately 195,000 cfs. On the latter date the total discharge was about 169,000 cfs. These surveys were less ambitious than the one of 1956. In the February run, current velocity measurements were made at boat stations F, G, H, I and J in the upper part of the Bay system; and salinity measurements were made at boat stations A, F, G, H, I and J, and shore stations 18 and 20 (see Figure 7.48); observations of tide were made at 11 shore stations. The March survey included current velocities and salinities measured at only 4 boat stations, G, H, I and K.

Model reproduction of prototype tidal ranges, elevations, and phases was considered satisfactory in both cases. For the 1956 survey, the maximum error observed in the model at the 23 gages was 0.4 feet prototype (0.004 feet, model). Current velocities were satisfactorily reproduced at the 11 control stations. The maximum difference between model and prototype absolute velocities was somewhat over one ft/sec. Examples of the low inflow verification are shown in Figure 7.49.

With the same roughness elements as the 1956 case, and an inflow of 195,000 cfs, the model results for 13-14 February were somewhat low in salinity and exhibited higher velocities, particularly in Suisun and San Pablo Bays, This was compensated for by reducing the inflows



TEST CONDITIONS

MEAN TIDE OF 21-22 SEPT 1956
FRESH-WATER INFLOW AT CHIPPS ISLAND=16,000 CFS
OCEAN SALINITY=33 PPT

Fig. 7.49 Example of physical model verification for low inflow conditions.

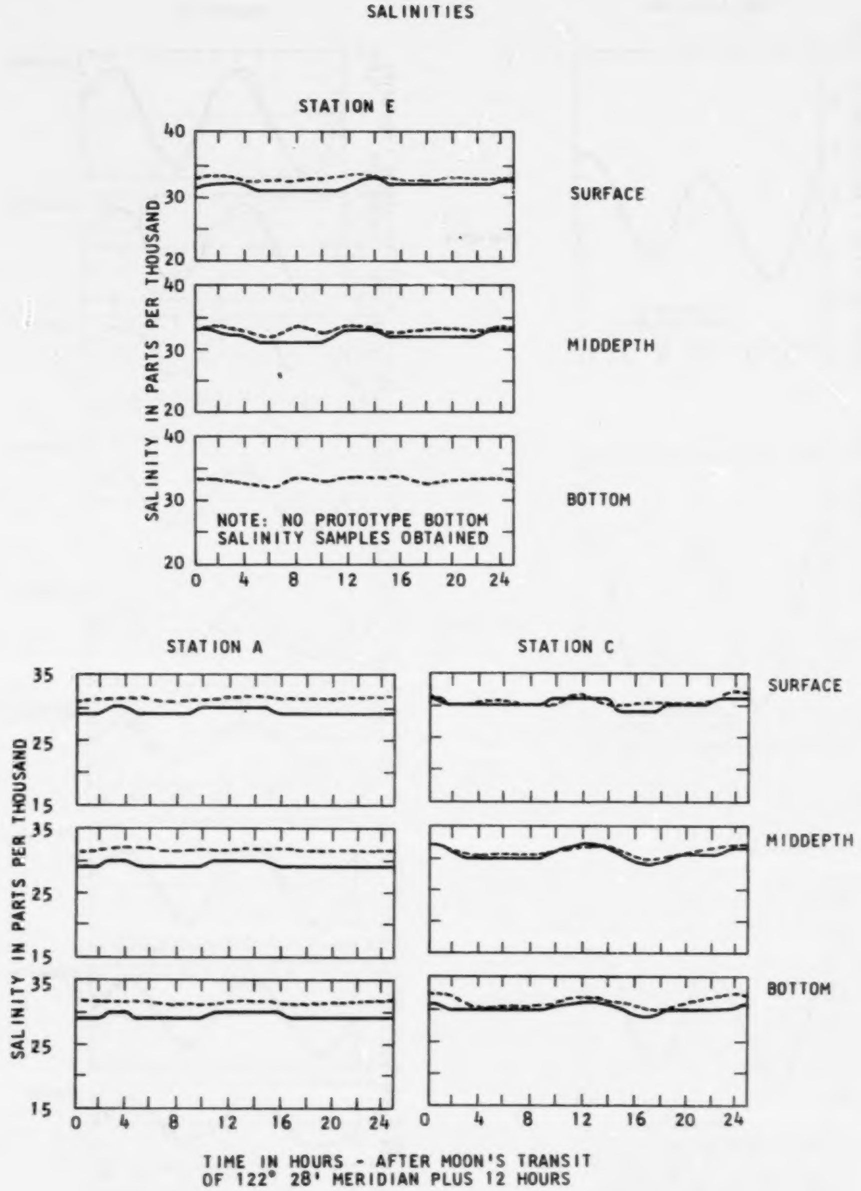
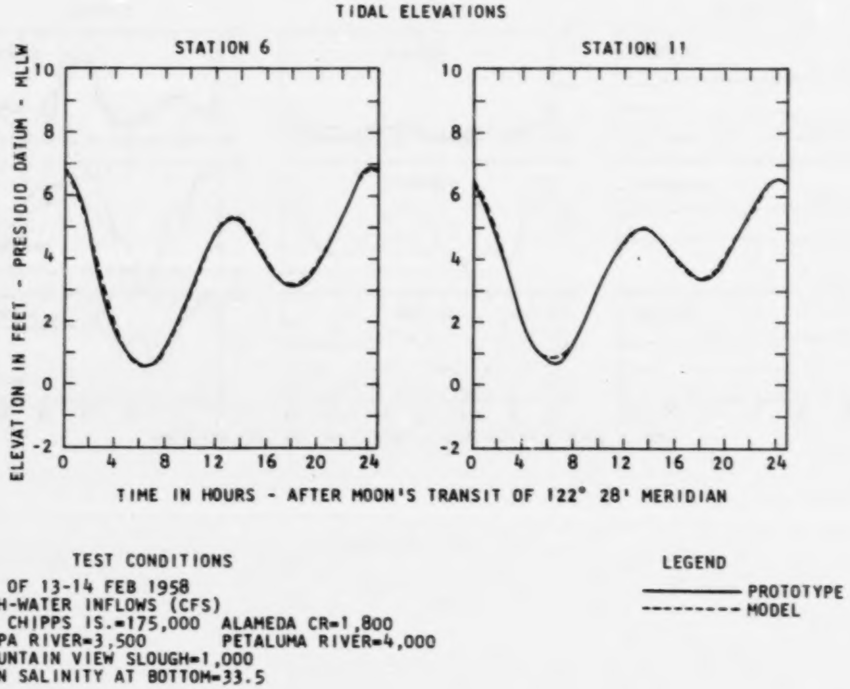


Fig. 7.49 Continued

to 185,300 cfs and making slight alterations in the roughness elements in the navigation channel of Suisun and San Pablo Bays. The alteration in the inflow was considered permissible due to the errors in estimating the prototype inflows, especially in that the effects of evaporation, transpiration, and consumption are not well accounted for. Examples of model-prototype comparisons for the high inflows are given in Figure 7.50.

4.2.2 Evaluation of the Effects of Solid Barriers on Hydraulics and Salinities

Much of the work performed by the Corps of Engineers and reported in USCE (1963) was directed at the evaluation of the influence of proposed barriers on the San Francisco Bay System. The barriers investigated and their approximate locations are shown in Figure 7.51. The barrier studies were conducted with two kinds of simulated tides: the approximate mean tide of 21-22 September 1956, for which the model was verified, and the spring tide of 13 September 1954. The former exhibited considerable diurnal inequality and the latter practically no inequality. The freshwater flows of the Sacramento and San Joaquin Rivers dicharged into Suisun Bay on 21-22 September 1956 and 13 September 1954 were considerably below the mean daily freshwater inflow (45,000 cfs) into the Bay system being 16,000 cfs and 7,000 cfs, respectively The purpose of the tests of solid barriers was to determine the effects of the barriers on the



TEST CONDITIONS
TIDE OF 13-14 FEB 1958
FRESH-WATER INFLOWS (CFS)
AT CHIPPS IS.=175,000 ALAMEDA CR=1,800
NAPA RIVER=3,500 PETALUMA RIVER=4,000
MOUNTAIN VIEW SLOUGH=1,000
OCEAN SALINITY AT BOTTOM=33.5

Fig. 7.50 Example of physical model verification for high inflow conditions.

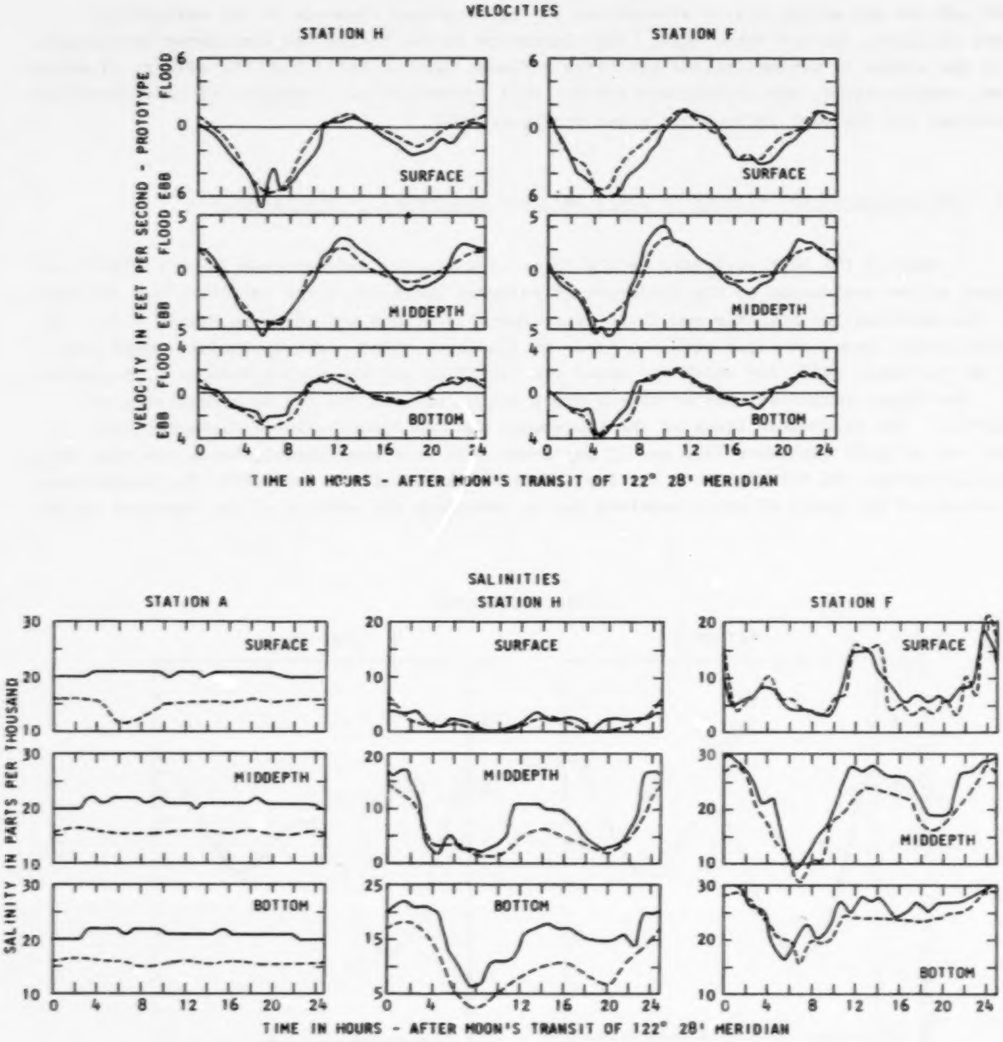


Fig. 7.50 Continued

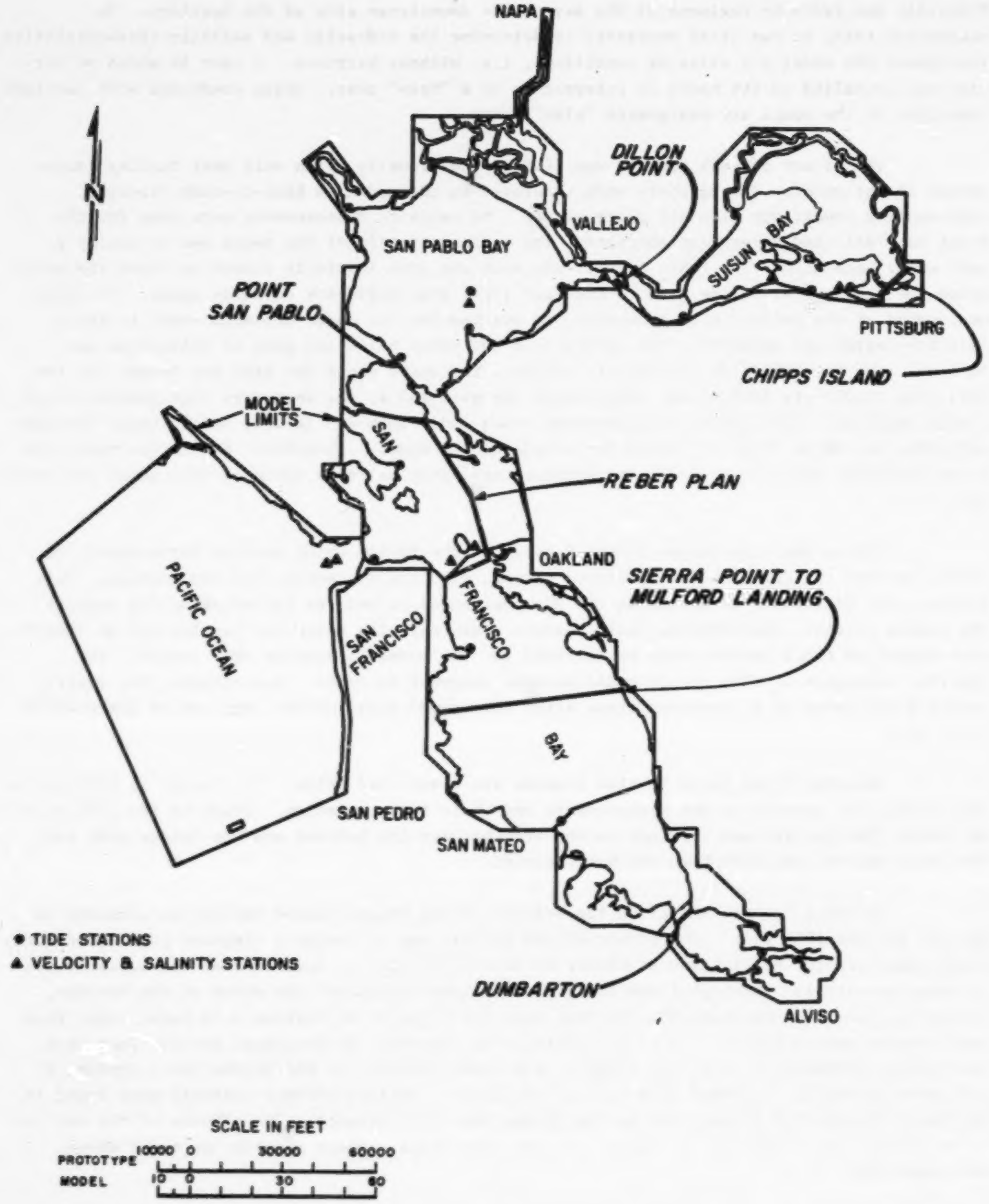

NAPA
DILLON POINT
VALLEJO
N
SAN PABLO BAY
SUISUN BAY
POINT SAN PABLO
PITTSBURG
CHIPPS ISLAND
MODEL LIMITS
SAN
REBER PLAN
OAKLAND
SIERRA POINT TO MULFORD LANDING
PACIFIC OCEAN
SAN FRANCISCO
FRANCISCO
BAY
SAN PEDRO
SAN MATEO
● TIDE STATIONS
▲ VELOCITY & SALINITY STATIONS
DUMBARTON
ALVISO
SCALE IN FEET
PROTOTYPE 10000 0 30000 60000
MODEL 10 0 30 60

Fig. 7.51 San Francisco Bay physical model, location map of barriers.

hydraulic and salinity regimens of the Bay on the downstream side of the barriers. To accomplish this, it was first necessary to determine the hydraulic and salinity characteristics throughout the model for existing conditions, i.e. without barriers. A test in which no barrier was installed in the model is referred to as a "base" test. Tests conducted with barriers installed in the model are designated "plan" tests.

The effect of each barrier was studied individually, with only that barrier implemented in the model. The barriers were simulated in the model as bank-to-bank closures, representing conditions with all gates closed. No salinity measurements were made for the Point San Pablo and Reber Plan Barriers. The basic operation of the tests was to employ a salt water gate across San Pablo Strait, and with the gate initially closed to flood the model below the gate and above the gate to the same level with different salinity water. The gate was opened as the primary tide generator was started and the model operated until a steady salinity regime was obtained. The salinity of the water below the gate at initiation was 30 o/oo. For the 1956 tide (16,000 cfs inflow), the water above the gate was fresh; for the 1954 tide (7,000 cfs inflow) the water above the gate and at the secondary tide generator was 5 o/oo salinity. This latter was necessary since under such low inflow, saline water intrudes well into the Delta which is beyond the bounds of the model. Therefore, the inflow had to be at an increased salinity in order to reproduce realistic salinity contours throughout the Upper Bay.

With either the Chipps Island Barrier or the Dillon Point Barrier implemented, no inflow reaches the Bay from the effective source, viz. the Sacramento and San Joaquin. This imposes some difficulty in operating the physical model as well as interpreting the results. The stable salinity distribution would produce ocean salinity below the barrier and an inordinate amount of tidal cycles would be required for the model to acquire this result. The physical relevance of this result would also be somewhat in doubt. Accordingly, the results reported are those of a transient state after twenty-odd tidal cycles, and are of qualitative value only.

Results of the solid barrier studies are summarized below. The reader is referred to USCE (1963) for details of the measurements and their interpretation. Study of the effects of the Reber Plan Barrier was confined to the area between the barrier and the Golden Gate and the ocean beyond, and therefore are not reported.

In Table 7.9 are indicated the effects of the Chipps Island Barrier on currents in the Bay for the 1956 tide. The effect of the barrier was to create a stagnant pool immediately downstream from the barrier and to reduce current velocities to Station I at the westerly end of Carquinez Strait. Average flood and ebb velocities throughout the depth at the barrier, Station K, were reduced about 97% (to less than 0.1 ft/sec); at Station J in Suisun Bay, they were reduced nearly 50% (to 1.2 to 1.7 ft/sec); at Station I in Carquinez Strait, they were practically unchanged (3.5 to 3.7 ft/sec); and from Station I to the Golden Gate, Station E, they were generally increased from 0.2 to 0.9 ft/sec. Maximum surface currents were found in San Pablo Strait (6.5 ft/sec) and in the Golden Gate (5.2 ft/sec). The effects of the barrier on salinities are summarized in Table 7.10 for both tides. These results, as noted above, are transient.

The effect of the Dillon Barrier on currents was to create a stagnant pool immediately downstream from the barrier and to reduce current velocities for a considerable distance downstream. Its effects on salinities are indicated in Table 7.11; once again, these represent a transient condition.

TABLE 7.9

Effects of Chipps Island Barrier on Current Velocities

Tide of September 21-22, 1956

(Average Velocities Throughout Depth in ft/sec)

Location	Station	Without Barrier		With Barrier		Change (ft/sec)	
		Flood	Ebb	Flood	Ebb	Flood	Ebb
Golden Gate	E	4.0	4.3	4.6	4.5	+0.6	+0.2
West of Treasure Island	C	3.3	3.4	3.1	2.9	-0.2	-0.5
San Pablo Strait	G	3.2	4.3	4.1	5.1	+0.9	+0.8
San Pablo Bay	H	2.3	3.9	3.0	3.7	+0.7	-0.2
Carquinez Strait	I	3.8	3.5	3.7	3.5	-0.1	0.0
Suisun Bay	J	2.0	3.1	1.2	1.7	-0.8	-1.4
Barrier Site	R	2.6	3.3	0.1	0.1	-2.5	-3.2

TABLE 7.10

Effects of Chipps Island Barrier on Salinities

(Average Salinities Throughout Depth in ppt)

Station	Tides							
	21-22 September 1956				13 September 1954			
	Without Barrier		With Barrier		Without Barrier		With Barrier	
	Max.	Min.	Max.	Min.	Max.	Min.	Max.	Min.
E Golden Gate	32.7	31.2	33.0	32.3	32.7	30.5	33.5	32.0
C West of Treasure Island	32.3	29.8	31.8	30.2	32.0	28.2	32.3	30.0
D East of Treasure Island	31.5	28.9	30.9	29.1	30.6	27.3	31.9	30.1
G San Pablo Strait	30.0	22.7	31.0	26.5	26.7	19.0	31.0	28.2
H San Pablo Bay	26.7	20.8	29.7	24.2	21.2	14.5	30.0	26.7
I Carquinez Strait	21.8	11.7	25.3	18.7	15.3	6.2	27.3	21.5
J Suisun Bay	9.8	1.5	16.0	12.8	5.5	4.5	20.5	17.8
R At Barrier	3.5	0.5	13.7	13.0	5.5	4.5	18.7	17.7

TABLE 7.11

Effects of the Dillon Point Barrier on Salinities

(Average Salinities Throughout Depth in ppt)

Station	Tides							
	21-22 September 1956				13 September 1954			
	Without Barrier		With Barrier		Without Barrier		With Barrier	
	Max.	Min.	Max.	Min.	Max.	Min.	Max.	Min.
E Golden Gate	32.7	31.2	33.2	32.2	32.7	30.5	32.0	31.5
C West of Treasure Island	32.3	29.8	33.5	31.3	32.0	28.2	31.5	30.7
G San Pablo Strait	30.0	22.7	31.2	28.0	26.5	19.0	30.7	27.8
H San Pablo Bay	26.7	20.8	29.2	26.8	21.2	14.5	29.3	27.5
P San Pablo Bay	24.7	16.8	28.0	26.0	-	-	-	-
I Carquinez Strait	21.8	11.7	28.2	26.3	15.2	5.7	27.7	26.7

The Point San Pablo Barrier was tested with the spring tide of 11-12 November 1958 and was found to cause a small increase in current velocities of less than 1.0 ft/sec in South Bay, and a reduction in Central Bay from the Golden Gate to the barrier. The maximum reduction occurred at the barrier, where flood and ebb were reduced to 0.6 ft/sec (reductions in flood and ebb of 2.6 and 3.3 ft/sec, respectively). Salinity measurements were not made.

The 1956 tide was used in the tests with the Sierra Point to Mulford Landing Barrier. As in the case of the barriers in the upper Bay system, the Sierra Point to Mulford Landing Barrier created a relatively stagnant pool adjacent to the barrier and for some distance downstream therefrom. At the barrier, velocities (averaged over the depth) were reduced to about 0.1 ft/sec (flood reduced 2.3 ft/sec, and ebb, 2.1 ft/sec). At Station C, west of Treasure Island, flood and ebb velocities were reduced to 0.7 and 1.0 ft/sec, respectively (reductions of 2.6 and 2.4 ft/sec). At Station E in the Golden Gate, flood and ebb velocities were reduced to 3.0 and 2.4 ft/sec, respectively (reductions of 1.0 and 1.9 ft/sec). Elsewhere throughout the Bay system, velocities were reduced or increased from 0.1 to 0.7 ft/sec. The effect of the barrier on the salinities in the Bay was slight with the greatest change in Suisun Bay and Carquinez Strait. The effects of this barrier are summarized in Table 7.12.

Dumbarton Barrier, the southernmost of the barriers examined, was tested with the 1956 tide. As might be anticipated, the barrier had little effect on either the currents or the salinities throughout the Bay system. The barrier created a stagnant pool which extended some distance from the barrier. At the barrier, the velocities were reduced to zero (reductions in flood and ebb of 3.0 and 2.3 ft/sec, respectively); at Station M, approximately midway between Dumbarton and San Mateo Bridges, flood and ebb were reduced to 0.3 and 0.2 ft/sec, respectively (reductions in flood and ebb of 1.9 and 1.5 ft/sec); and from Station M to Station C, west of Treasure Island, reductions amounted to 0.5 to 1.0 ft/sec. Between the Golden Gate and Station I in Carquinez Strait, the maximum reduction was 0.6 ft/sec; and in a few areas, flood or ebb velocities were increased from 0.1 to 0.2 ft/sec. The greatest change in salinity

TABLE 7.12

Effects of the Sierra Point to Milford Landing Barrier on Salinities

Station	Maximum Salinities (Parts Per Thousand)			Minimum Salinities (Parts Per Thousand)		
	Base Test	Plan Test	Change	Base Test	Plan Test	Change
E	32.7	33.5	+0.8	31.2	32.3	+1.1
C	32.3	31.8	-0.5	29.8	30.0	+0.2
G	30.0	30.0	0.0	22.7	23.7	+1.0
H	26.7	26.8	+0.1	20.8	22.0	+1.2
I	21.8	21.5	-0.3	11.7	14.8	+3.1
J	9.8	12.2	+2.4	1.5	3.3	+1.8
K	2.0	3.2	+1.2	0.5	1.0	+0.5

occurred at Station I in Carquinez Strait, where the average maximum salinity throughout the depth was reduced to 2.8 ppt. At all other stations, the maximum and minimum salinities were generally reduced from 0.4 to 1.7 ppt.

An interesting aspect of the investigation of the solid barriers in the physical model is that it presented an opportunity to compare the results of the physical model with those of an analog model. An earlier report by Harder (1957) described the results of calculating tidal range with and without the Chipps Island Barrier using an analog computer. In this study, a sinusoidal tide of period 12.4 hours was employed which corresponded very closely to the tide of 13 September 1954. The hydraulic model results for the 1954 tide with and without the Chipps Island Barrier are compared with analog results in Table 7.13. The differences in these results are attributed to a number of factors, for example, the use in the electric analog of a pure sinewave tide with a 12.4-hour period, whereas in the hydraulic model the actual tide with period of 24.8 hours was used (with some differences in the ranges of the first and second 12.4-hour periods). Another suggested source of the disagreement is the extreme difficulty of accurately determining the roughness of the prototype channel and areas outside of the channel for use in the analog model.

4.2.3 Application of Dye Releases

The physical model has been employed on a number of occasions to provide information on the dispersive characteristics of the Bay using flourescent dye as a tracer. The Corps, of course, has conducted extensive studies of dye releases in the model (USCE 1963), and additional studies are reported in O'Connell and Walter (1963), Bailey *et al*. (1966), Lager and Tchobanoglous (1968), and McCullough and Vayder (1968). The principal objective of the dye releases performed by the Corps (1963) was to provide information on the dispersion patterns of different wastes released into the San Francisco Bay System, both under existing conditions and with the implementation of the proposed barriers. All tests were run for an inflow of 16,000 cfs from the Sacramento and San Joaquin Rivers, except for the instances where barriers

TABLE 7.13

Comparison of Results of Electric Analog and Hydraulic Model

(Effect of the Chipps Island Barrier
on the Tide of September 13, 1954)

Station	Electric Analog Tidal Range in Feet			Hydraulic Model Tidal Range in Feet		
	No Barrier	With Barrier	Increase In Feet	No Barrier	With Barrier	Increase In Feet
Presidio	5.35	--	--	5.50	5.40	-0.10
Selby[(a)]	5.20	6.70	1.50	5.80	6.35	0.55
Eckley	5.10	7.30	2.20	5.70	6.95	1.25
Benicia[(b)]	5.10	8.20	3.10	5.40	7.30	1.90
Roe Island[(a)]	4.70	8.90	4.20	4.80	8.00	3.20
Nichols	4.50	9.20	4.70	4.55	8.35	3.80
Chipps Island	3.90	9.30	5.40	4.10	8.50	4.40

(a) Hydraulic model data were taken from HHW and LLW profiles from nearby gages, since there are no fixed tide gages at these locations.

(b) Station 20 at Martinez (across the Strait from Benicia) used in hydraulic model.

restricted flow from these two rivers. Dye release points and the barriers tested are shown in Figure 7.52. Within this series of tests, 18 dye release points were employed and all base tests (i.e., no barriers) were conducted using the approximate mean tide of 21-22 September 1956. Each test run was carried for 20 or 40 tidal cycles per release depending on the particular case. Dye concentrations were obtained for contour plots after 1, 3, 5, 10, 15 and 20 cycles of the 20-cycle tests, and also after 30 and 40 cycles for the 40-cycle tests. The quantities of dye released depended upon the expected dispersal characteristics in the vicinity of release points and the particular test duration; that is, shorter tests and areas with slower flushing characteristics required smaller amounts of dye. In most cases, the dye was released over one tidal cycle (14.9 minutes in the model), approximately a slug release. Both continuous flourometer readings and discrete samples were obtained during each test run.

The results for the Sierra Point to Roberts Landing Barrier is indicative of this work. In Figure 7.53 are shown the dye contours resulting from an injection at point "G" without the barrier after 3, 5 and 10 cycles. Under these (base) conditions, that part of South San Francisco Bay north of the barrier site exhibits better circulation of tidal currents, and consequently more rapid dispersion and flushing action, than that part of the Bay south of the barrier site. In Figure 7.54 are shown the corresponding plots with the solid barrier from Sierra Point to Roberts Landing. Dye releases at Point "G" with the barrier showed action in South Bay north of the barrier to be considerably more sluggish than without the barrier, dispersion and flushing action occuring more slowly with high concentrations of dye persisting

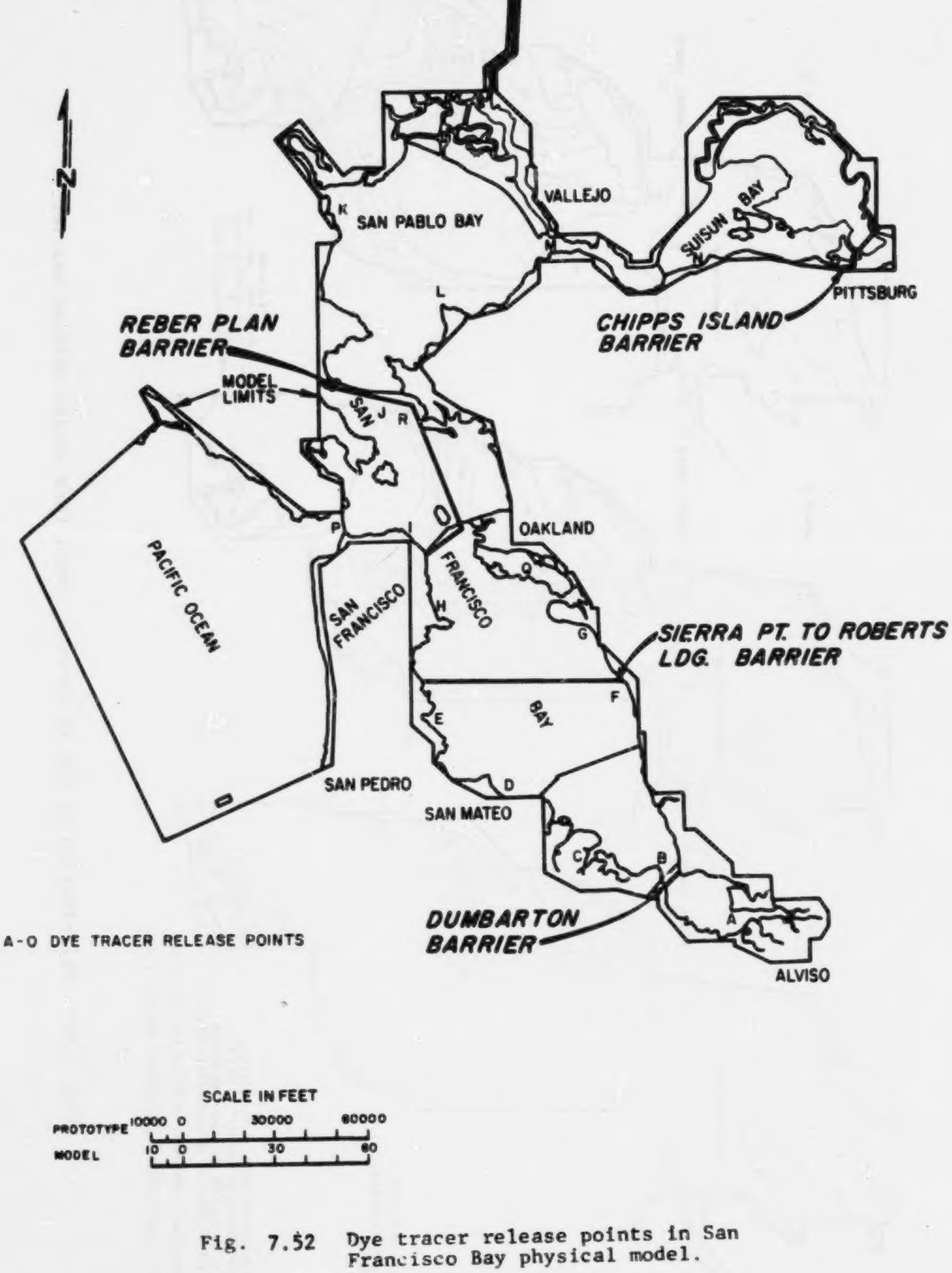

N
NAPA
VALLEJO
K
SAN PABLO BAY
SUISUN BAY
PITTSBURG
L
CHIPPS ISLAND BARRIER
REBER PLAN BARRIER
MODEL LIMITS
SAN
J
R
P
I
O
OAKLAND
PACIFIC OCEAN
SAN FRANCISCO
FRANCISCO
H
G
SIERRA PT. TO ROBERTS LDG. BARRIER
F
E
BAY
D
SAN PEDRO
SAN MATEO
C
B
A
DUMBARTON BARRIER
ALVISO
A-O DYE TRACER RELEASE POINTS
SCALE IN FEET
PROTOTYPE 10000 0 30000 60000
MODEL 10 0 30 60

Fig. 7.52 Dye tracer release points in San Francisco Bay physical model.

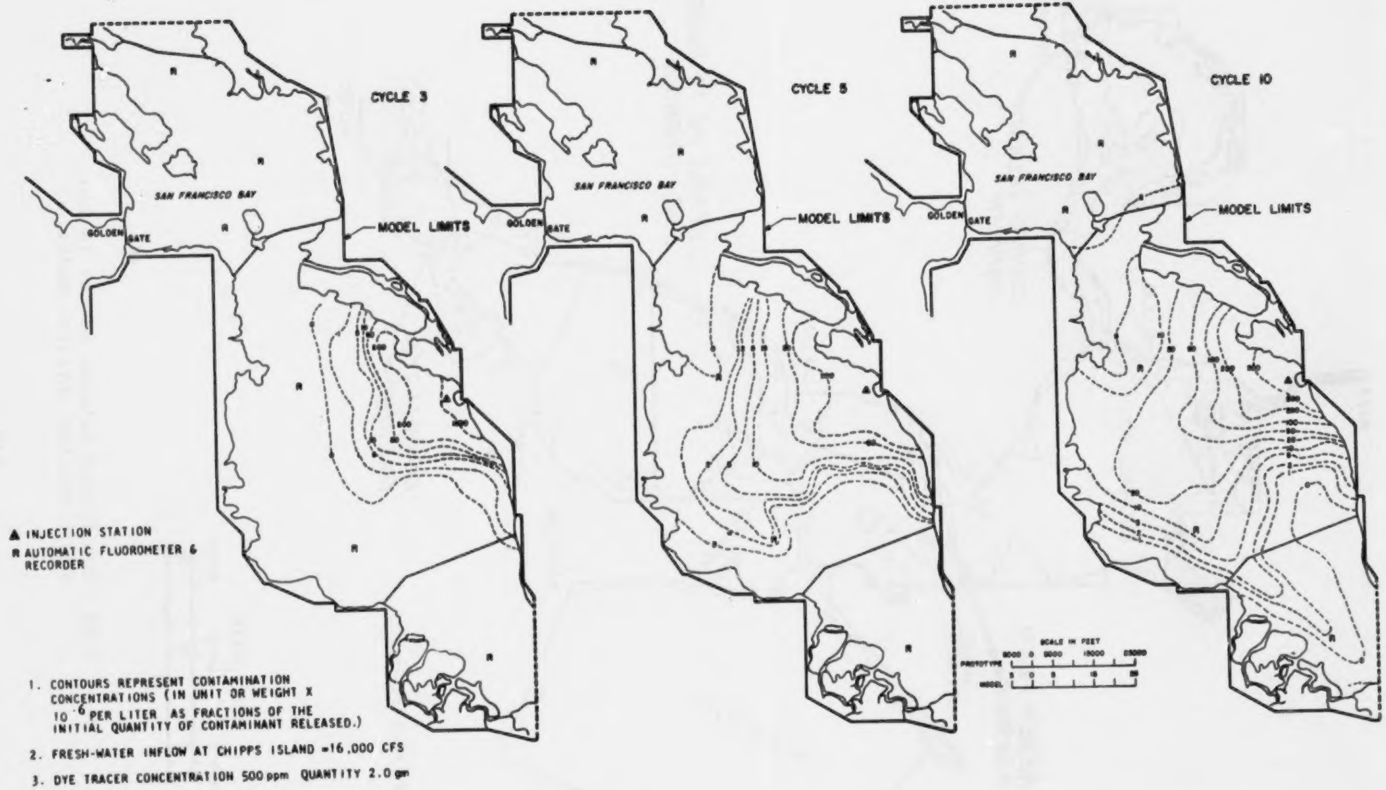

CYCLE 3
CYCLE 5
CYCLE 10
SAN FRANCISCO BAY
GOLDEN GATE
MODEL LIMITS
R
▲ INJECTION STATION
R AUTOMATIC FLUOROMETER & RECORDER
1. CONTOURS REPRESENT CONTAMINATION CONCENTRATIONS (IN UNIT OR WEIGHT X 10⁻⁶ PER LITER AS FRACTIONS OF THE INITIAL QUANTITY OF CONTAMINANT RELEASED.)
2. FRESH-WATER INFLOW AT CHIPPS ISLAND =16,000 CFS
3. DYE TRACER CONCENTRATION 500 ppm QUANTITY 2.0 gm
SCALE IN FEET
PROTOTYPE
5000 0 5000 15000 25000
MODEL
5 0 5 15 25

Fig. 7.53 Distribution of dye in physical model (HHW Slack) without barrier.

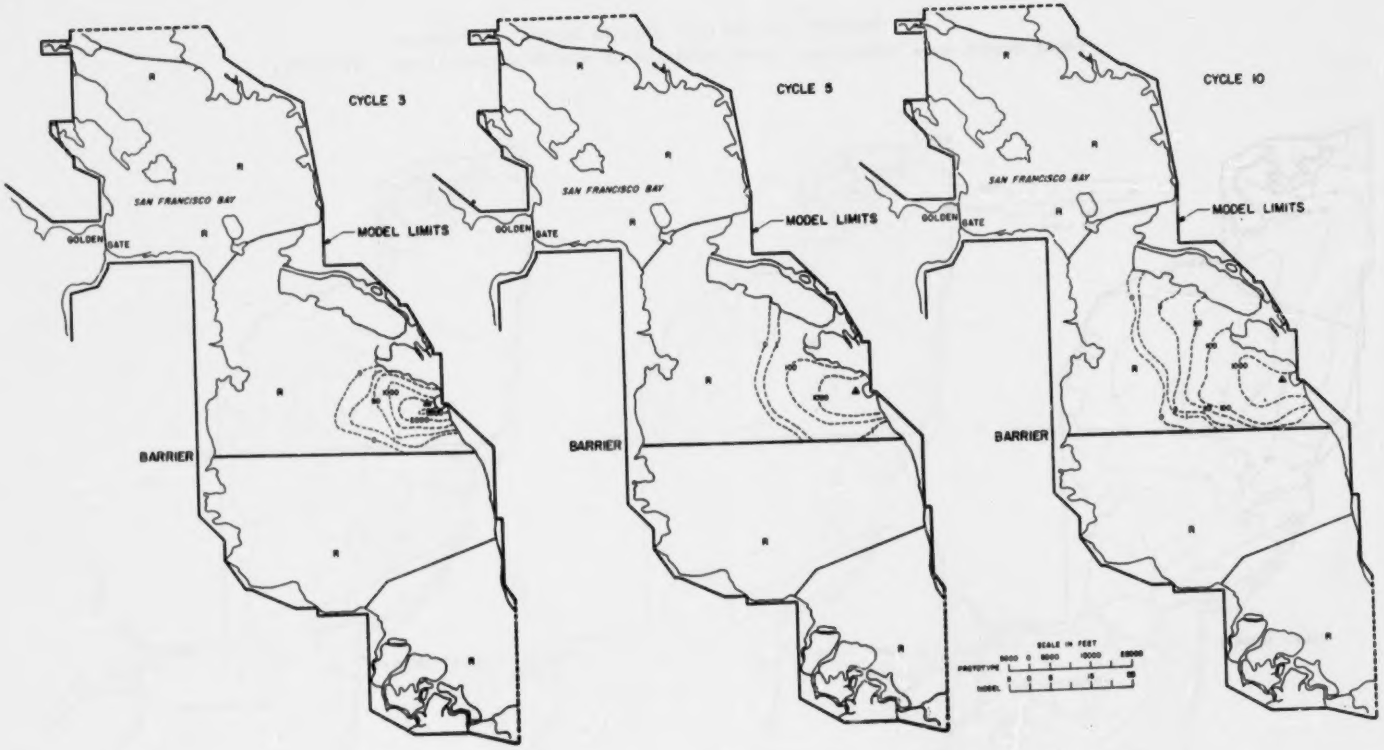

CYCLE 3
CYCLE 5
CYCLE 10
MODEL LIMITS
SAN FRANCISCO BAY
GOLDEN GATE
BARRIER
R
SCALE IN FEET
PROTOTYPE
MODEL
5000
0
5000
10000
15000

Fig. 7.54 Distribution of dye in physical model (HHW Slack) with Sierra Point to Roberts Landing Barrier.

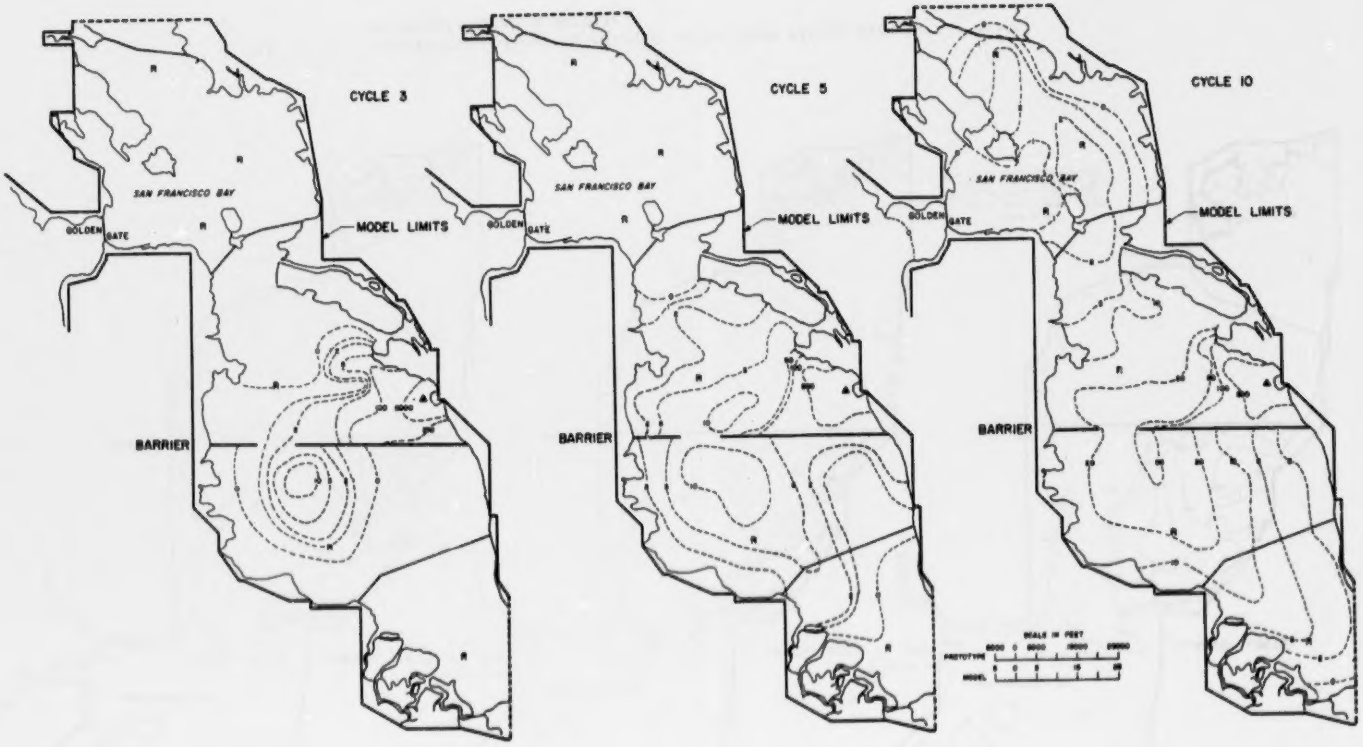

CYCLE 3
CYCLE 5
CYCLE 10
SAN FRANCISCO BAY
GOLDEN GATE
MODEL LIMITS
BARRIER
R
SCALE IN FEET
PROTOTYPE
8000 0 8000 16000 24000
MODEL
8 0 8 16 24

Fig. 7.55 Distribution of dye in physical model (HHW Slack) with Sierra Point to Roberts Landing Barrier with partial opening.

for longer periods of time. The results were quite different with a 10,000 foot navigation opening in the Barrier at the ship channel. These results are displayed in Figure 7.55. The addition of the Sierra Point Tidal Barrier with a 10,000 foot gate caused dramatic changes in the dispersion patterns in South Bay and improved the dispersion and flushing characteristics of this bay, as is evident by the faster dispersals of dye in all directions from the points of release of the dye. The improvement was due to the increase in current velocities and turbulence created by the navigation openings especially in deep water both upstream and downstream from the barrier. In general, there was a spread of dye in all directions at least equal to or greater than that in the base test. The movement of the dye was predominantly toward the west parallel to the barrier (rather than along the shore in the north-south direction). Once the dye reached and entered the navigation opening in the barrier, the increased current velocities moved the dye southward in deep water faster than in the base test and the overall progression in South Bay was more to the south than to the north.

The studies reported in O'Connell and Walter (1963), Bailey et al. (1966) and Lager and Tchobanoglous (1968) were conducted in a similar manner, except that the results were extended to be interpreted in terms of a nonconservative tracer by applying a decay factor to the station history curves. In Bailey et al. (1966), comparisons were made between dye measurements in the prototype and the model to verify the latter's ability to represent mixing phenomena in the Bay. Release and sampling points in the prototype are shown in Figure 7.56. The model was operated with 16,000 cfs inflow, approximately that of the prototype. The dye concentration histories at three stations for model and prototype are displayed in Figure 7.57. The prototype values have been multiplied by 10^8, the mass scale factor, and have been corrected for dye loss using an empirical exponential fit to the observed time histories. In general, the dye concentrations in the model varied from about twice the prototype values near Chipps Island to almost equal the prototype values in Suisun Bay. The discrepancies are suggested to be due to boundary effects in the model or variations between the constant model tide and the varying prototype tide. In Figure 7.58 are shown steady-state dye dispersion curves, corrected to represent a conservative tracer, obtained from four different injection points at 16,000 cfs. It can be seen that the concentrations are sensitive to the location of the discharge point in Suisan Bay but not nearly so much in San Pablo Bay. Model tests were also performed to evaluate the influence of flow on the steady-state concentrations, as is exemplified by Figure 7.59.

4.3 DIGITAL COMPUTER MODEL

The numerical hydraulic-water quality model for San Francisco Bay described in this section was developed principally by Water Resources Engineers, Inc. (WRE), through a series of contract agreements with the PHS and later FWPCA. The model effectively represents two spatial dimensions in the horizontal, and is general in that it can be applied to any estuarine system sufficiently well mixed in the vertical. Indeed, it has been applied to Sydney Harbor (Australia), San Diego Bay and the Columbia River, among others. However, it was originally developed for San Francisco Bay and most of the computational experience with the model has been obtained in the Bay system, so it is appropriate to undertake the discussion of the model in this section.

4.3.1 Theory and Computational Framework

The computation of currents and of the distribution of substance (i.e., the water quality) are undertaken separately. Fundamentally, the computations are independent, but

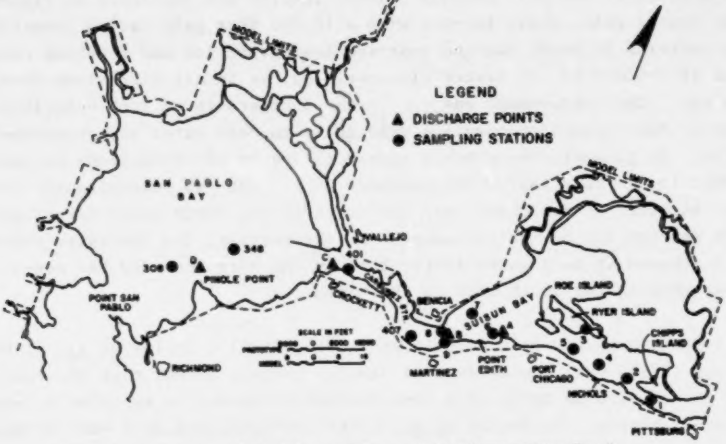

MODEL LIMITS
LEGEND
DISCHARGE POINTS
SAMPLING STATIONS
SAN PABLO BAY
VALLEJO
401
C
348
308
D
PINOLE POINT
POINT SAN PABLO
RICHMOND
CROCKETT
CARQUINEZ STR.
BENICIA
SUISUN BAY
407
6
8
9
7
A
MARTINEZ
POINT EDITH
PORT CHICAGO
ROE ISLAND
RYER ISLAND
CHIPPS ISLAND
5
3
4
2
1
NICHOLS
PITTSBURG
SCALE IN FEET
PROTOTYPE
MODEL

Fig. 7.56 Location of sampling stations and discharge points for dye dispersion tests in the San Francisco Bay System. From T. E. Bailey, C. A. McCullough and C. G. Gunnerson, Mixing and Dispersion Studies in San Francisco Bay, Proc. ASCE, 92, No. SA5 (Oct., 1966), pp. 23-45. Used with permission of the American Society of Civil Engineers.

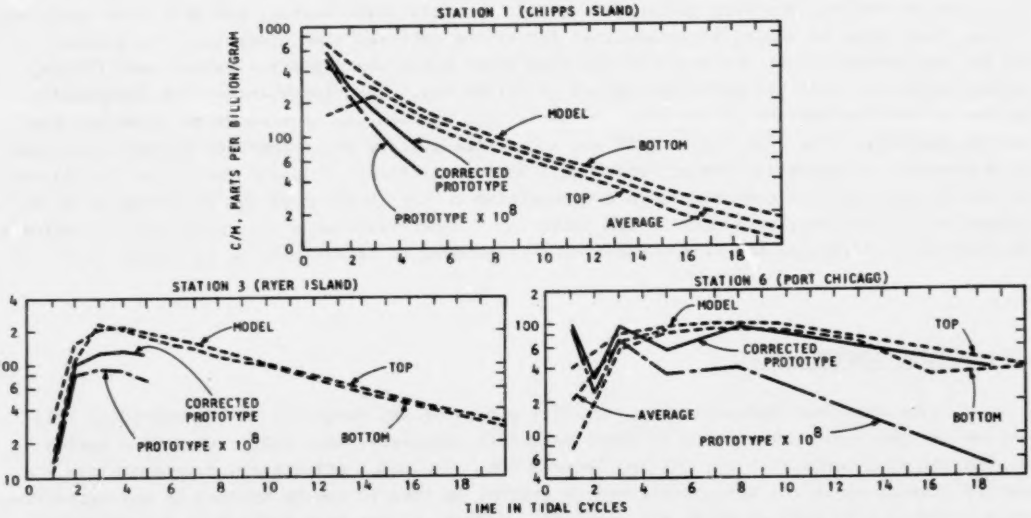


Fig. 7.57 **Verification of the hydraulic model by comparison with prototype dye dispersion patterns. From T. E. Bailey, C. A. McCullough and C. G. Gunnerson, Mixing and Dispersion Studies in San Francisco Bay, Proc. ASCE, 92, No. SA5 (Oct., 1966), pp. 23-45. Used with permission of the American Society of Civil Engineers.**

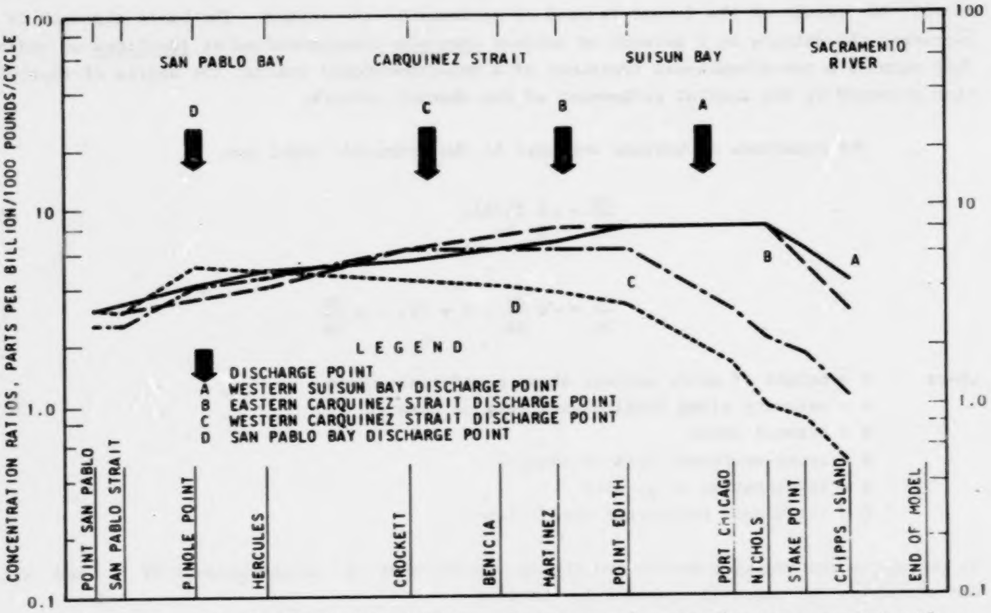


Fig. 7.58 Longitudinal distribution of conservative steady-state concentrations at HHW Slack resulting from four separate discharges at 16,000 cfs inflow. From T. E. Bailey, C. A. McCullough and C. G. Gunnerson, Mixing and Dispersion Studies in San Francisco Bay, Proc. ASCE, 92, No. SA5 (Oct., 1966), pp. 23-45. Used with permission of the American Society of Civil Engineers.

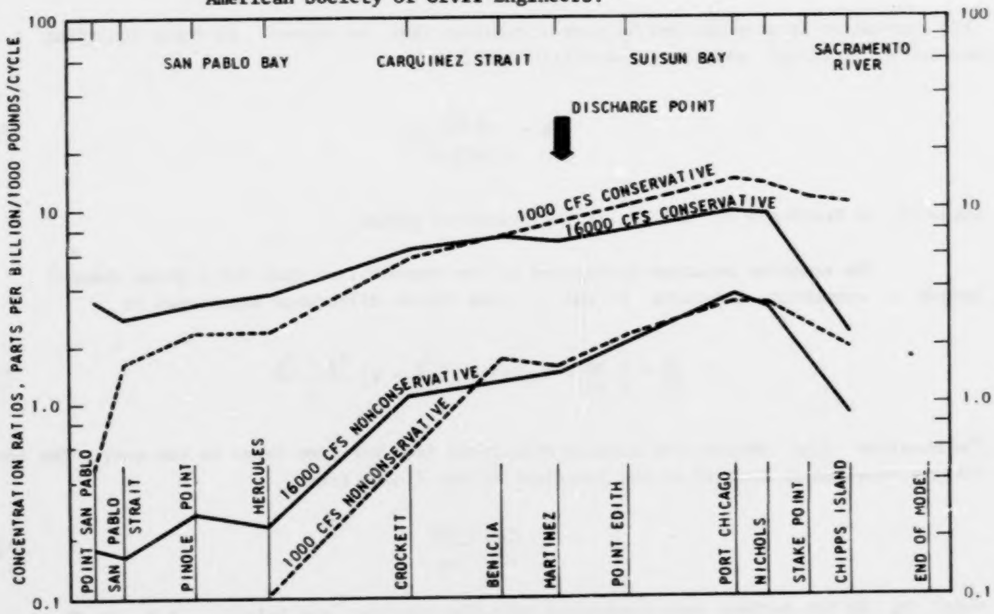


Fig. 7.59 Comparison of concentration ratios of constituents discharged at Martinez into 1,000 and 16,000 cfs inflows. From T. E. Bailey, C. A. McCullough and C. G. Gunnerson, Mixing and Dispersion Studies in San Francisco Bay, Proc. ASCE, 92, No. SA5 (Oct., 1966), pp. 23-45. Used with permission of the American Society of Civil Engineers.

usually the result of the former is used as an input to the latter. The basic approach is to represent the estuary as a network of uniform channels interconnected at junctions or nodes. This permits a one-dimensional treatment of a two-dimensional system, the degree of approximation governed by the spatial refinement of the channel network.

The equations of motions employed in the hydraulic model are

$$\frac{\partial H}{\partial t} = -\frac{1}{B}\frac{\partial (vA)}{\partial x} \tag{7.5}$$

$$\frac{\partial v}{\partial t} = -v\frac{\partial v}{\partial x} - K v |v| - g\frac{\partial H}{\partial x} \tag{7.6}$$

where H = height of water surface above a reference datum
v = velocity along longitudinal axis of channel
B = channel width
A = cross-sectional area of channel
g = acceleration of gravity
K = frictional resistance coefficient

By using the continuity equation and the assumption that B is independent of t and x, one can transform the momentum equation to the form

$$\frac{\partial v}{\partial t} = \frac{v}{A}\frac{\partial A}{\partial t} - K v |v| + \left(\frac{v^2 B}{A} - g\right)\frac{\partial H}{\partial x} \tag{7.7}$$

This expression is computationally more convenient than the former. In these equations K denotes a frictional resistance coefficient given by

$$K = \frac{g n^2}{2.208 R^{4/3}} \tag{7.8}$$

where n is Manning's "n" and R is the hydraulic radius.

The momentum equation is applied to the channels, so that for a given channel length L connecting junctions i and j, the finite-difference expression is

$$\frac{\Delta v}{\Delta t} = \frac{v}{A}\frac{\Delta A}{\Delta t} - K v|v| + \left(\frac{v^2 B}{A} - g\right)\frac{H_j - H_i}{L} \tag{7.9}$$

The notation $\Delta/\Delta t$ denotes the divided difference from one time level to the next. The continuity equation is applied at the junctions in the finite form

$$\frac{\Delta H}{\Delta t} = \frac{\Sigma_n Q_n}{A_s} \tag{7.10}$$

where A_s is the surface area associated with the junction (see below). $\Sigma_n Q_n$ is the (algebraic) sum of the flows into the junction, not only from the channels, but also from discharges, withdrawals and other external effects. The variables v, B, A and K are associated with the channels, and H and A_s are associated with junctions.

Figure 7.60 is an example of how a channel-junction network might be established for both one-dimensional and two-dimensional systems. Mean depths are obtained from standard bathymetric charts or equivalent sources. If the natural system is essentially one-dimensional, e.g. a system of channels, the mean width and surface area can be estimated from maps. For a two-dimensional body, the system of centroids (the points of intersection of the perpendicular bisectors of the channels) determines both the widths and surface areas as indicated in Figure 7.60. The cross-sectional area of every channel is the product of its width and depth. Two networks for the same system, Suisun Bay, are shown in Figures 7.61 and 7.62, the former from WRE (1968) and the latter from Orlob et al. (1967).

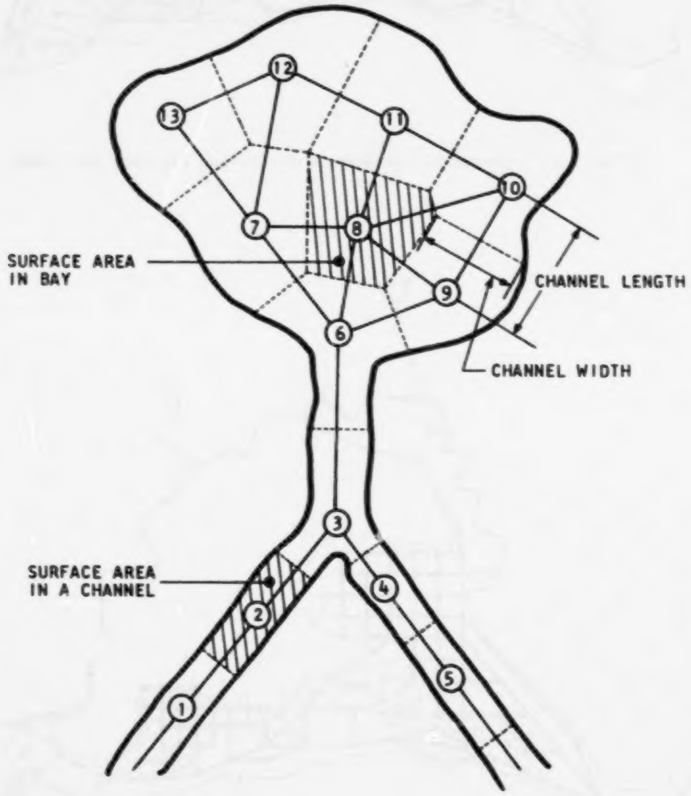


Fig. 7.60 Calculation of Surface Area.

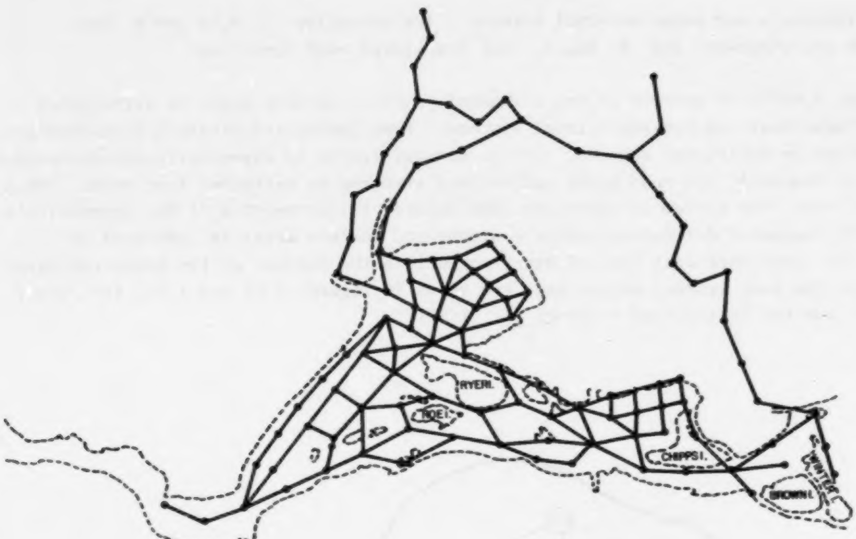

RYER I.
ROE I.
CHIPPS I.
BROWN I.
WINTER I.

Fig. 7.61 Computational Network for Suisun Bay from WRE (1968).

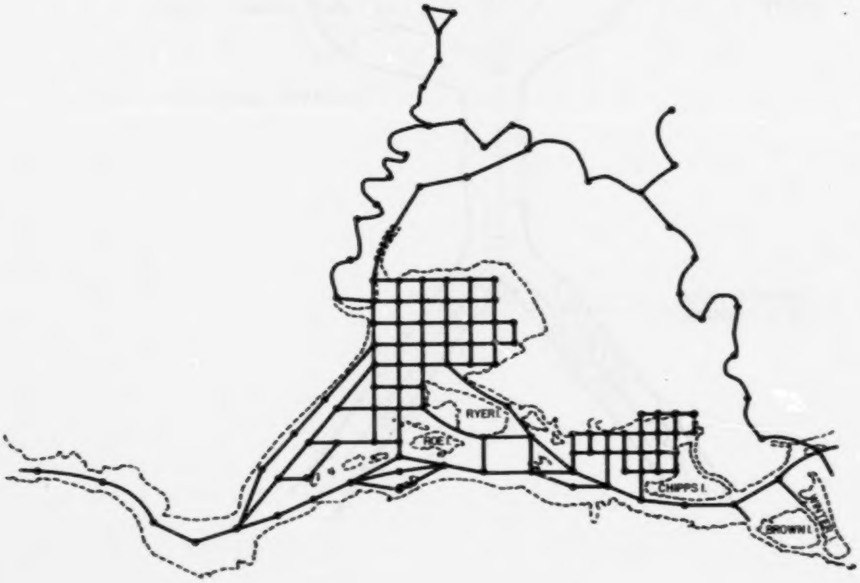

RYER I.
ROE I.
CHIPPS I.
BROWN I.
WINTER I.

Fig. 7.62 Computational Network for Suisun Bay from Orlob et al (1967).

The solution of these equations is performed in an explicit manner using a modified Runge-Kutta method, which calculates the variables at the temporal half step $t + \Delta t/2$ then uses these half-step values in computing the variables at $t + \Delta t$. Details of the program operation may be found in Feigner and Harris (1970) and WRE (1968); mathematical aspects of general Runge-Kutta methods are summarized in Todd (1962), Sections 9.2-9.5.

The transport per unit area per unit time of a conservative constituent in a channel is assumed to be given by

$$T = \frac{\partial M}{\partial t} = Qc - AE\frac{\partial c}{\partial x} \tag{7.11}$$

where Q is the flow in the channel, c the concentration and E the dispersion coefficient. The corresponding finite-difference expression is

$$\Delta M = Av\hat{c} - EA\frac{c_j - c_i}{L} \tag{7.12}$$

The quantity $\hat{c}$ is a representation of the concentration advected in the channel and is chosen to provide the "best" numerical behavior (e.g. numerical mixing, stability, and accuracy). In Orlob _et al_. (1967) the most satisfactory methods were found to be

$$\hat{c} = \frac{3c_i + c_j}{4}$$

$$\hat{c} = \begin{cases} \frac{1}{2}(c_i + c_j) + \frac{u}{2}(c_i - c_j) & c_i > c_j \\ c_i & c_i < c_j \end{cases}$$

where i designates the upstream concentration. The former was used extensively.

At a given junction, the contributions to the mass for each channel ΔM_n after the integration time Δt are determined from Equation (7.12) by a modified Runge-Kutta method. Thus the mass at the junction at $t + \Delta t$ is given by

$$M_{t+\Delta t} = M_t + \Sigma_n \Delta M_n \tag{7.13}$$

The volume is similarly advanced in time (see WRE 1968) and the concentration at $t + \Delta t$ is found to be

$$c = \frac{M_{t+\Delta t}}{V_{t+\Delta t}}$$

Extension to a nonconservative constituent is handled simply by incrementing $M_{t+\Delta t}$, after its computation by (7.12), according to the expressions for the source and sink processes. Thus, the mass of a first-order decaying substance at $t + \Delta t$ is incremented by the amount

$$\Delta M = -K_1 V c_t \Delta t$$

where K_1 is the reaction rate.

4.3.2 Model Application and Verification

The model described in the preceding section has been operated extensively in many forms for the San Francisco Bay system. A version used extensively by WRE for the Bay-Delta Water Quality Control Program employed a coarse network of 250 junctions and 325 channels for the entire Bay system, in comparison to the preceding representation of Suisun Bay (Figure 7.61) which alone utilized 135 junctions and around 200 channels.

Figure 7.63 exemplifies the ability of the hydraulic model to produce the tidal stages when the boundary tide is input at Benecia (see Figure 7.68). An example of the calculation of salinity distribution with this model is given in Figure 7.64. In this case there is a dynamic change in the chloride distribution during a one-month period. The following inputs were used:

1. Average July stream inflows and qualities.
2. Average July export values for the USBR pumping plants at Tracy and the Contra Costa Canal.
3. Initial chloride conditions (mean tidal values).
4. Average municipal and industrial flows.
5. An average July 1963 tide for the hydraulic model boundary at the Golden Gate.
6. A constant chloride value of 18,000 ppm for the quality boundary at the Golden Gate.

The hydraulic model was operated for three 25-hour tidal cycles in order to obtain a dynamic equilibrium. The computed net Delta outflow was 5,190 cfs, which represents a moderately high Delta summer outflow. The dynamic water quality model was operated for thirty-one 25-hour tidal cycles using the output from the hydraulic model. In Figure 7.64 are plotted salinities for the 31st tidal cycle along with the historical values of July 1, 1963, and July 31, 1963. The empirical data for July 1 were used as initial conditions in the model calculation. The curves represent the salinity gradient from the Golden Gate into the Delta. The model results compare favorably with the observed concentrations, particularly with regard to the gradients, and represent well the effect of salinity intrusion into the Delta.

Examples of the results of the fine grid model for the San Pablo-Suisun-Delta system are presented in Figures 7.65 through 7.69. Chlorinity predictions were made for two periods, July and September 1955, the former representing a period of salinity intrusion in the prototype and the latter, a period of salinity repulsion. Inputs to the model were daily river inflows, tide stage at Point Orient, exportations, mean monthly agricultural consumption, mean monthly evaporation, and municipal and industrial withdrawals and discharges. The net Delta outflow at Chipps Island was ca. 1,570 cfs in July and 5,540 cfs in September. Boundary conditions at Point Orient are shown in Figure 7.65. The hydraulic model results were in excellent agreement with the predictions in the tide tables for these periods. A comparison between the net flows calculated by the model and those predicted by the California Department of Water Resources for the two periods is given in Table 7.14. Again the agreement is good. The chlorinity boundary conditions for July (Figure 7.65) were increased by 2,250 mg/l after 27 days of operation to approximate the increase of salinity at the boundary. Similarly the chlorinity boundary values for September were decreased by 890 mg/l after 15 days of operation. The results of the chlorinity calculations for July and September for selected stations are displayed in Figure 7.66 and 7.67 along with empirical data for the corresponding periods. It is apparent that the agreement is quite good.

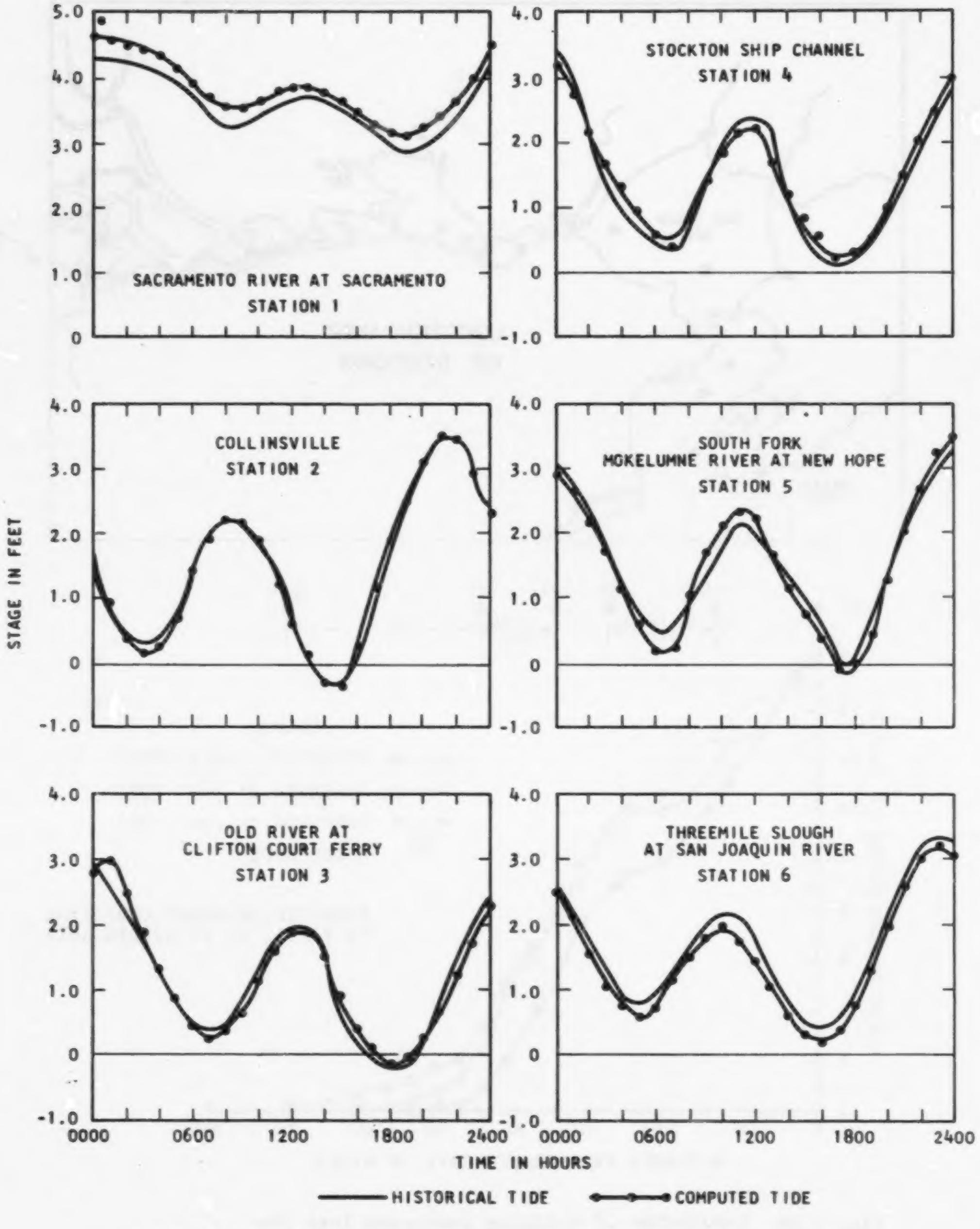


Fig. 7.63 Comparison of computed and observed tidal stages at selected locations in the Delta, 13 July 1959. After Kaiser Engineers (1969).

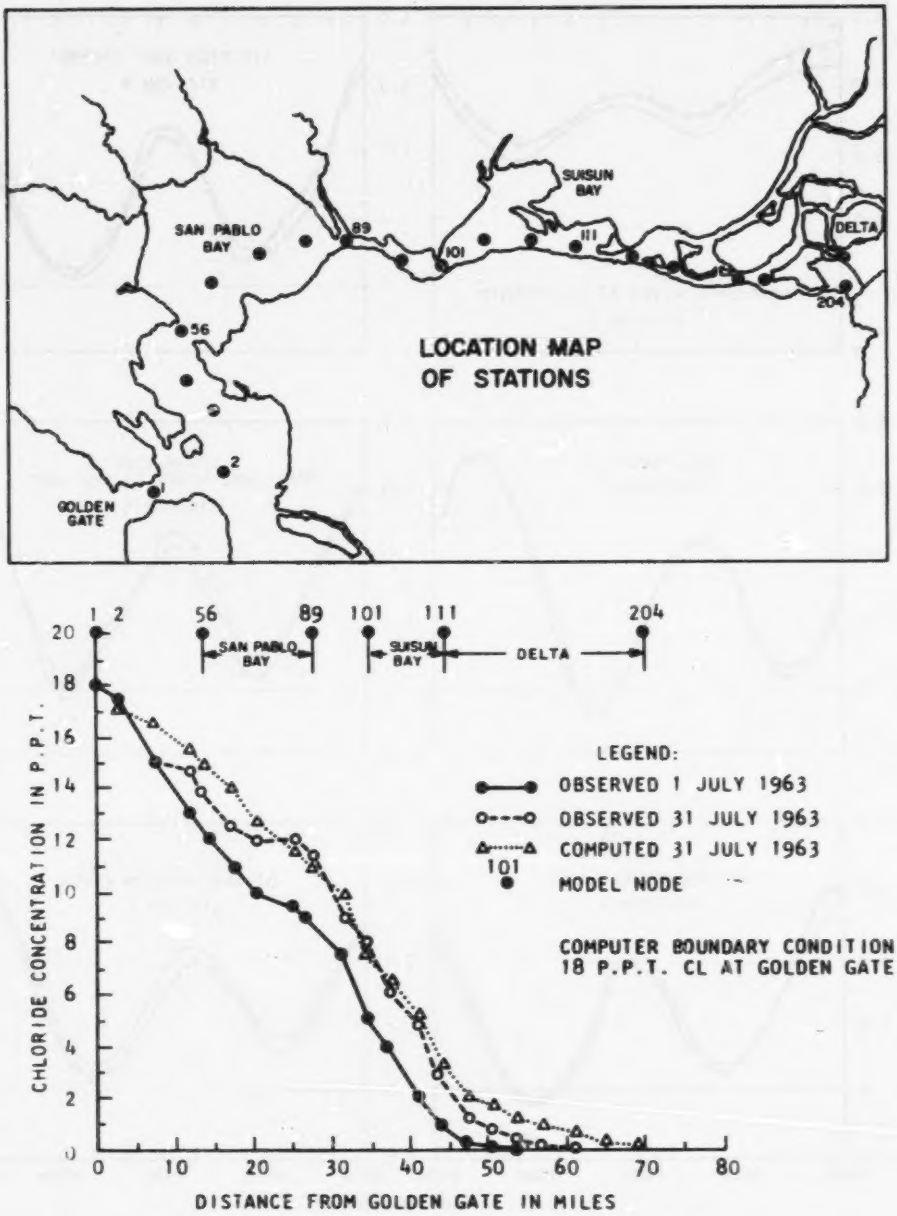


Fig. 7.64 Simulation of salinity intrusion into the Bay-Delta system dynamic water quality model Period 1 July to 31 July 1963. After Kaiser Engineers (1969).

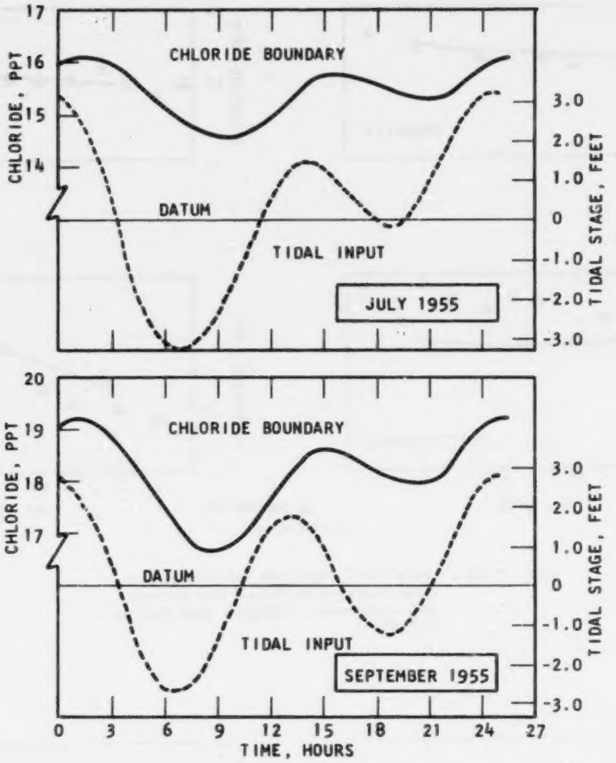


Fig. 7.65 Specified Boundary Conditions - July and September 1955 Chloride in San Francisco Bay-Delta. **After Feigner and Harris (1970).**

TABLE 7.14

Comparison of Predictions by the California Department of Water Resources and by FWPCA Numerical Model of Net Flows in Delta Channels From Feigner and Harris (1970)

Channel	July 1955		September 1955	
	DWR Prediction* (cfs)	FWPCA Model (cfs)	DWR Prediction* (cfs)	FWPCA Model (cfs)
Sac. River @ Sac.	8990**	8990**	9841**	9841**
Sutter Slough	1550	1539	1750	1811
Steamboat Slough	820	670	1000	795
Delta Cross-Channel	2950	2916	3100	3177
Georgiana Slough	1850	1561	1950	1755

* Empirical relationship

** Specified

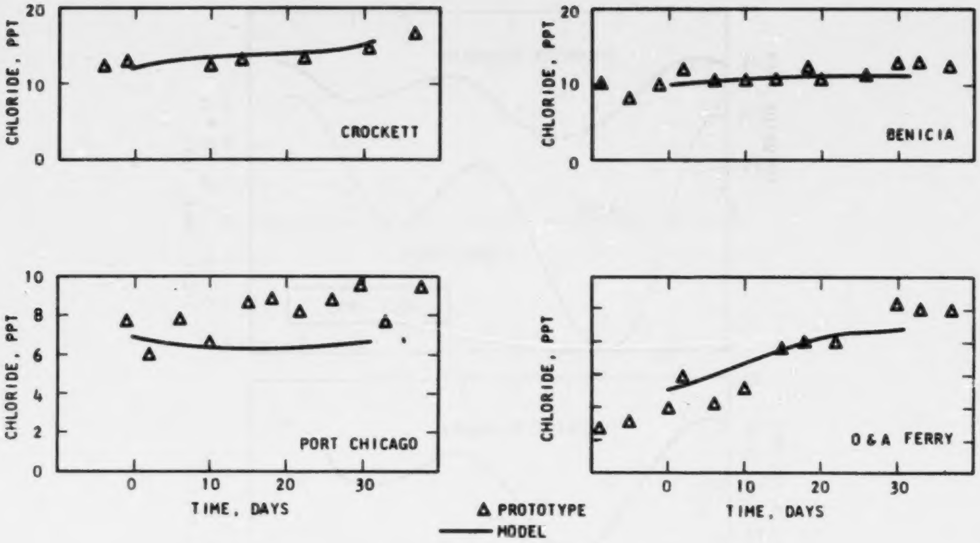


Fig. 7.66 July 1955 Chloride concentration histories--San Pablo and Suisun Bay Stations. Feigner and Harris (1970).

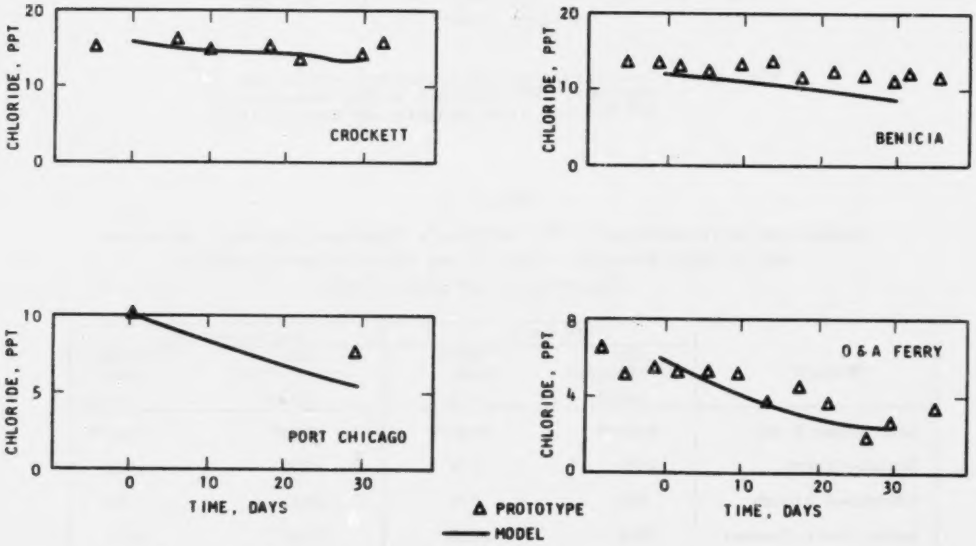
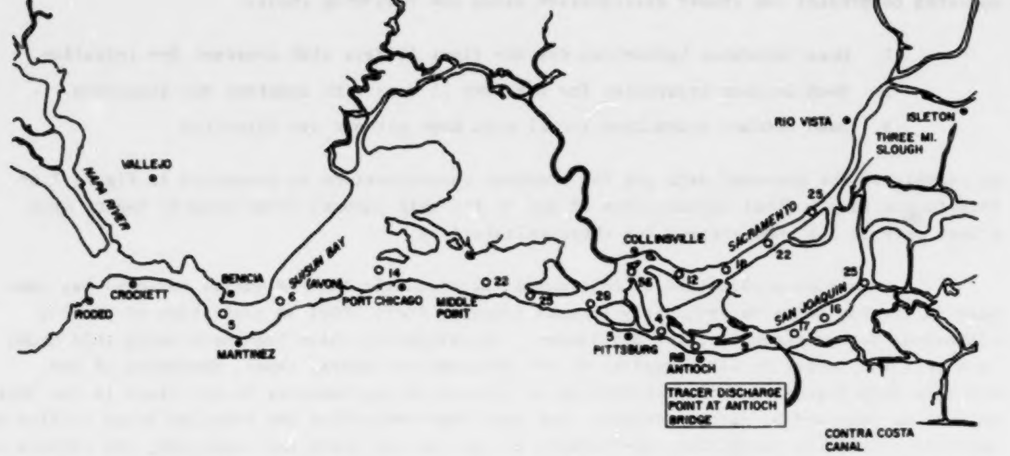


Fig. 7.67 September 1955 Chloride concentration histories--San Pablo and Suisun Bay Stations. Feigner and Harris (1970).



VALLEJO
NAPA RIVER
RODEO
CROCKETT
BENICIA
5
MARTINEZ
6
SUISUN BAY
(AVON)
14
PORT CHICAGO
MIDDLE POINT
22
25
29
COLLINSVILLE
15
5
4
5
PITTSBURG
ANTIOCH
12
18
22
SACRAMENTO
25
RIO VISTA
ISLETON
THREE MI. SLOUGH
25
SAN JOAQUIN
16
17
TRACER DISCHARGE POINT AT ANTIOCH BRIDGE
CONTRA COSTA CANAL

Fig. 7.68 Study Area with Tracer Sampling Stations. Feigner and Harris (1970).

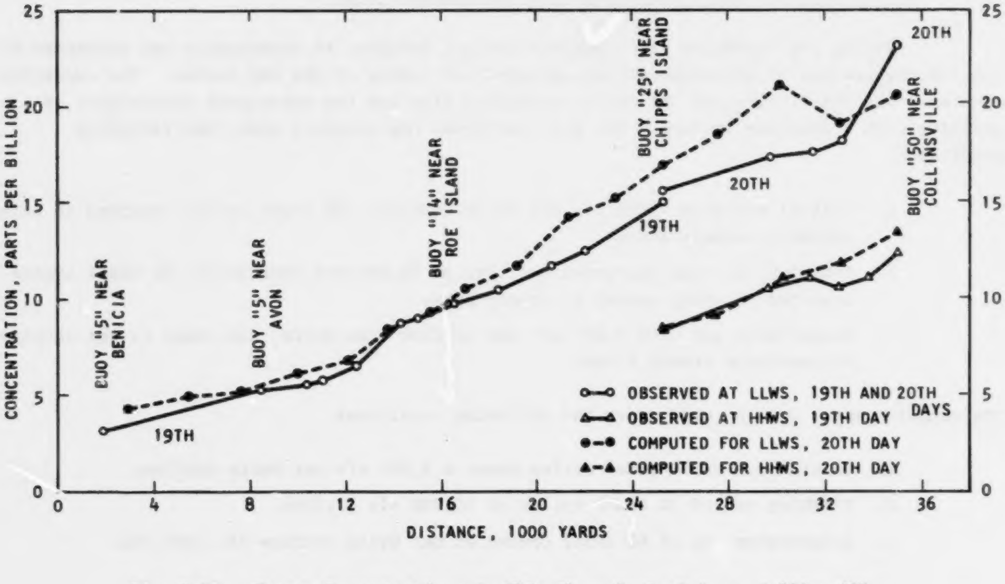


Fig. 7.69 Tracer Concentrations in Ship Channel--Benicia to Collinsville. Feigner and Harris (1970).

FWPCA performed an extensive dye release experiment in the Suisun Bay-Delta area in 1966, releasing Rhodamine WT continuously for 21 days from the Antioch Bridge and performing fluorometric measurements through the duration and for five weeks following the release. The point of discharge and the measuring stations are shown in Figure 7.68. The FWPCA model was operated to predict the tracer distribution using the following inputs:

1. Mean September hydraulics for the first 10 days with constant dye injection.
2. Mean October hydraulics for the next 11 days with constant dye injection.
3. Mean October hydraulics for 21 more days without dye injection.

An example of the measured data and the computed concentrations is presented in Figure 7.69. This is the longitudinal distribution of dye in the ship channel after roughly twenty days. A loss rate of 3.4% was assumed for these calculations.

Extensive application of this model (particularly the WRE coarse network) has been made in the Bay-Delta Water Quality Program (Program Staff 1969) in evaluation of problem situations for management of the Bay system. Investigations have been made using this model to assess the impact on water quality of the proposed peripheral canal, deepening of the Stockton Ship Channel and the restriction or closure of the entrance to Old River in the Delta, as well as proposed barriers. Studies have been made concerning the required Delta outflow to maintain acceptable salinities, the effects of various BOD loads and locations, the effects of relative toxicity of treated municipal and industrial wastes, and the efficacy of various local and regional systems of waste transport and disposal. Figure 7.70 is the result of an example calculation illustrating the effect of location on the concentrations resulting from a 10^6 lb/day load of a conservative constituent.

4.3.3 Comparison of Physical Model and Digital Computer Model

During the Bay-Delta Water Quality Control Program, an opportunity was presented to compare the results of the mathematical and physical models of the Bay system. The condition simulated was the flushing of the Bay by increased flow and the subsequent reintrusion of salinity with a decrease in flow. The physical model was operated under the following conditions:

1. Initial run with 2,000 cfs net Delta outflow; 120 tidal cycles required to bring system to steady state.
2. Flushing run with increased net flow of 30,000 cfs from Delta; 60 tidal cycles required to bring system to steady state.
3. Reintrusion run with 2,000 cfs net outflow from Delta; 114 tidal cycles required to reacquire steady state.

The computer model was operated under the following conditions:

1. Initial run of 10 tidal cycles under a 3,000 cfs net Delta outflow.
2. Flushing run of 30 tidal cycles at 30,000 cfs outflow.
3. Reintrusion run of 60 tidal cycles at net Delta outflow of 3,000 cfs.

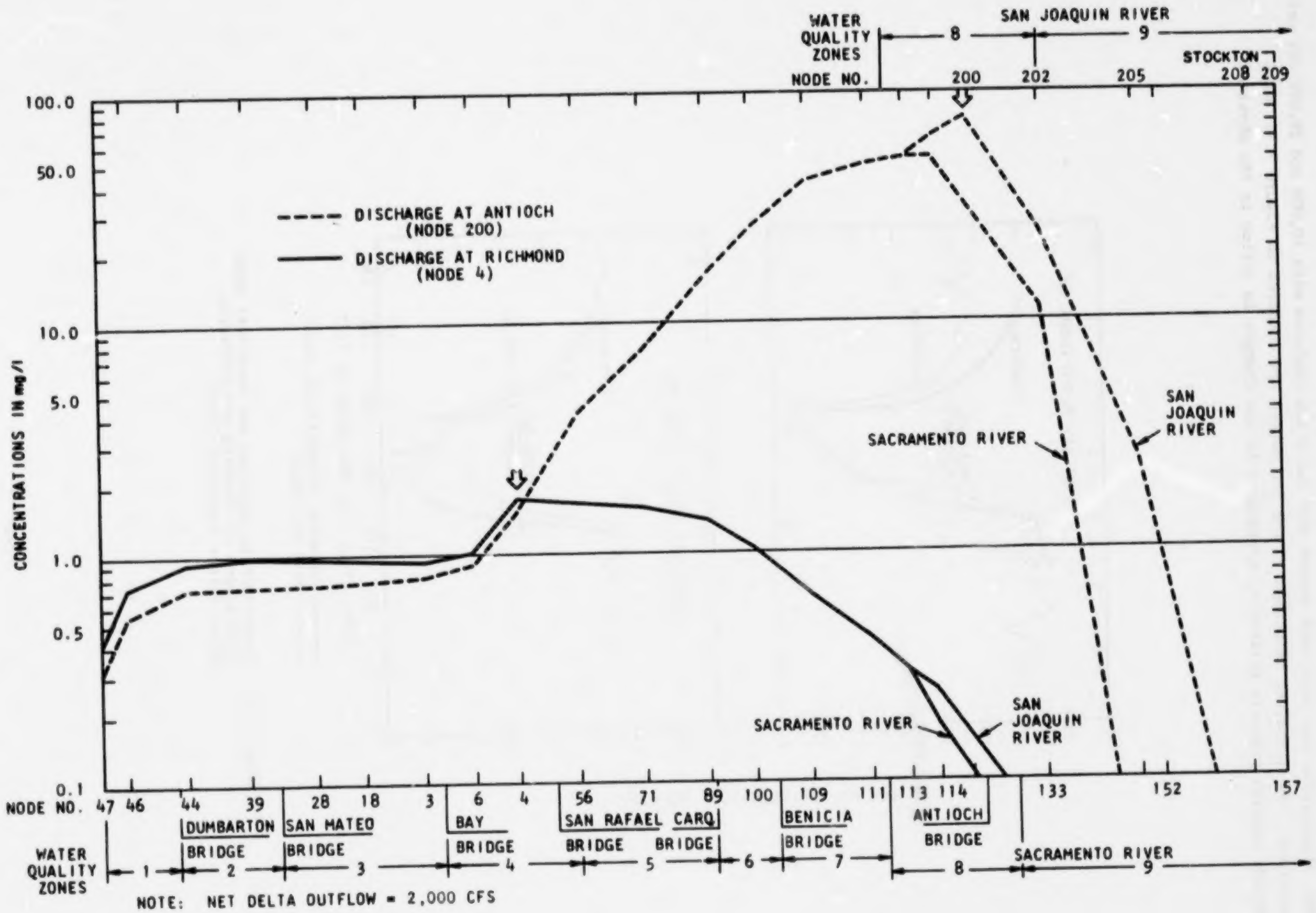


Fig. 7.70 Computed concentrations resulting from 10^6 lbs/day discharge at two different locations. After Program Staff (1969).

Two other simulations were also made except that run 2 was replaced with 10,000 and 20,000 cfs net Delta outflows. The transient responses of the two models are compared in Figure 7.71, with the computer results properly shifted to correspond to the changes in inflow in the physical model.

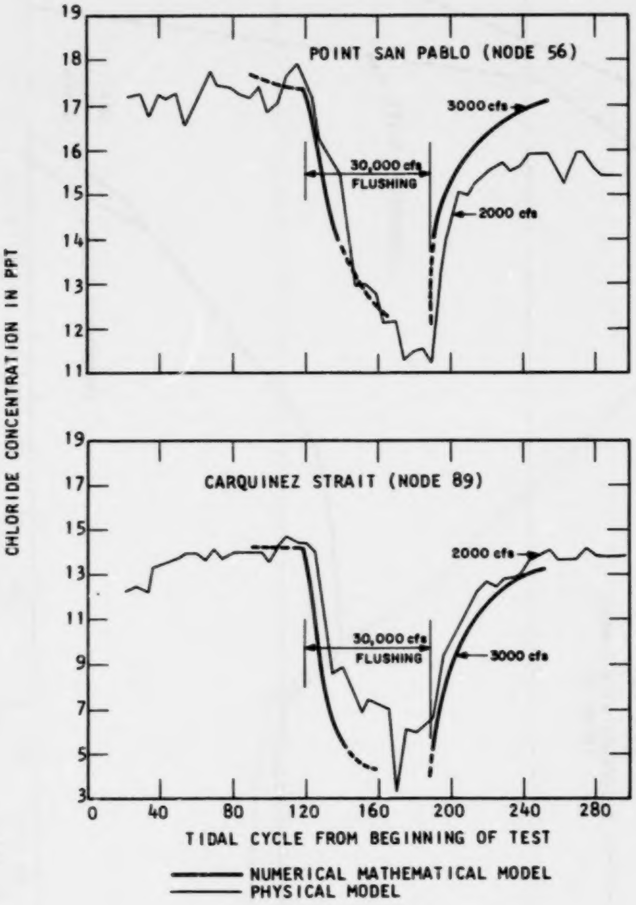


Fig. 7.71 Comparison of physical and numerical model simulations of flushing and intrusion. After Kaiser Engineers (1969).

5. GALVESTON BAY

Galveston Bay is the largest bay on the Texas Coast and is considered to be the most important, both economically and ecologically. The Bay is approximately 520 square miles in surface area (Figure 7.72) and includes the Port of Houston, Texas' most important commercial port. Moreover, the Bay provides receiving water for the wastes of the vast urban-industrial complex of the Houston area, and in this capacity has played an important part in the economy and continued growth of the region. The Bay system receives waste discharges from domestic and industrial sources, natural runoff, the Trinity River, San Jacinto River, Buffalo Bayou and the Houston Ship Channel, and various other small tributaries. The major source of industrial waste is the industrial complex located along the Houston Ship Channel above Baytown, estimated (Gloyna and Malina 1964) to average in excess of 200 million gallons per day. The commercial fishing industry in Galveston Bay is the most extensive and prolific along the Texas Gulf Coast, both by poundage and value. Furthermore, Galveston Bay hosts a diversity of aquatic life, and it is estimated that the Bay is the nursery grounds for approximately 80% of the total fishery product taken from the Gulf of Mexico along the Texas Coast (Curington et al. 1966).

Galveston Bay is typical of many of the estuaries along the Gulf Coast, in that the bay is shallow (average depth of 8 feet) and is nearly separated from the Gulf by barrier islands. The tidal range in the bay is small, one to two feet, and both water levels and currents are greatly influenced by wind. The Houston Ship Channel is maintained from Bolivar Roads to Morgan Point at a project depth of 40 feet, and continues up Buffalo Bayou some 25 miles to the Houston Turning Basin. Several other dredged channels traverse the Bay.

Galveston Bay has been characterized (Carter 1970) as an estuary in crisis, whose productivity and ecological functions are in immediate danger due to the combined effects of area development, e.g. waste disposal, shell dredging, freshwater diversion and upstream damming. Concern with this deterioration of the Bay's quality has brought about the strengthening of regulatory agencies to cope with these problems and the initiation of extensive research programs to provide a basis for regulation.

Within the last five years models have come into extensive use as predictive tools for water quality of Galveston Bay. (Prior to this physical models had been applied for problems of shoaling, harbor design and dredging, and limited mathematical models had been developed, such as the work of Urban and Masch 1966 based on an extension of the tidal prism approach of Ketchum 1951.) The models principally employed for water quality studies are a physical model operated by the Corps of Engineers Waterways Experiment Station and the mathematical models developed (or currently under development) by the Galveston Bay Project.

5.1 GALVESTON BAY PROJECT MATHEMATICAL MODELS

The Galveston Bay Project has been initiated by the Texas Water Quality Board and is basically directed toward the development of a comprehensive management program by which a suitable water quality level in the Bay can be determined and maintained with consideration for the many demands on the Bay resources. The Galveston Bay Project (GBP) has been the focal

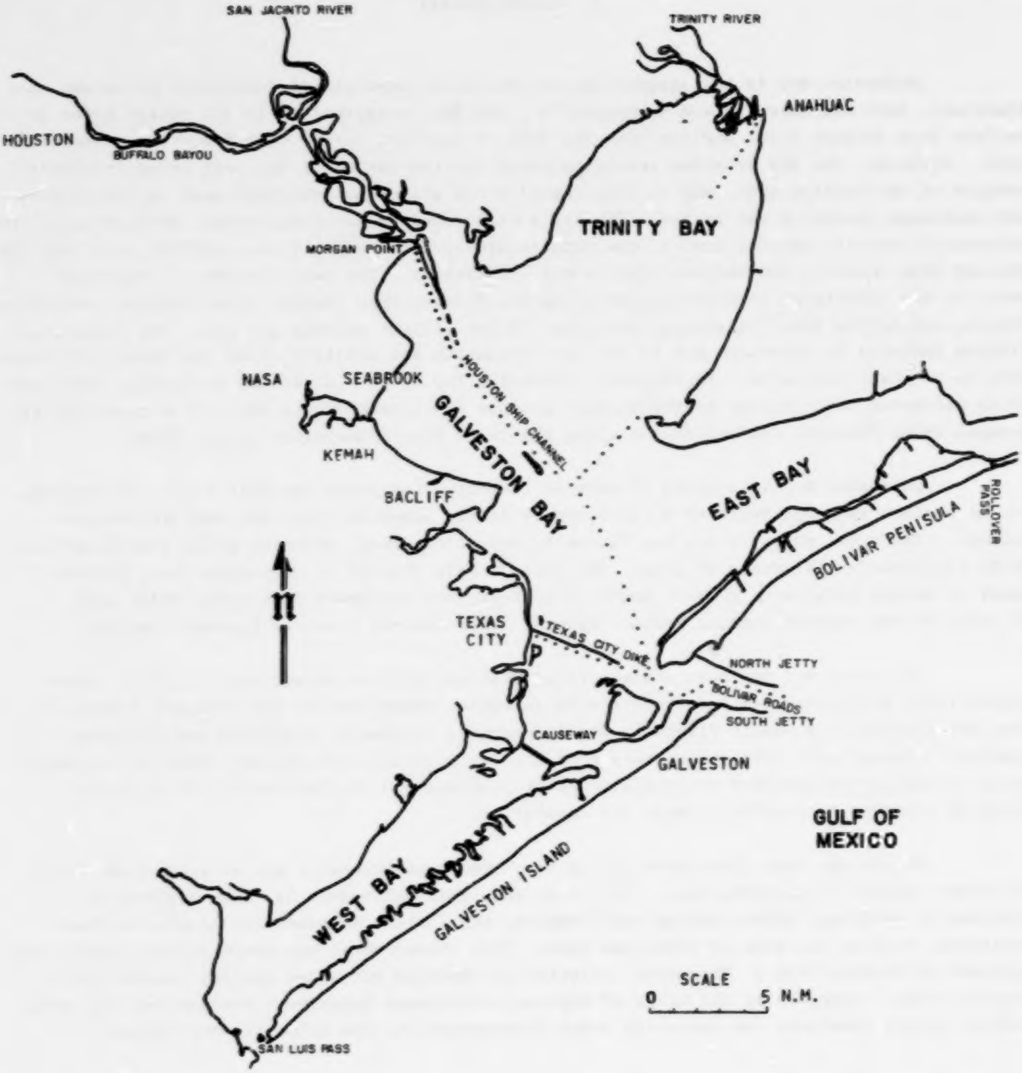

SAN JACINTO RIVER
TRINITY RIVER
ANAHUAC
HOUSTON
BUFFALO BAYOU
TRINITY BAY
MORGAN POINT
HOUSTON SHIP CHANNEL
NASA
SEABROOK
GALVESTON BAY
KEMAH
BACLIFF
EAST BAY
ROLLOVER PASS
BOLIVAR PENISULA
n
TEXAS CITY
TEXAS CITY DIKE
NORTH JETTY
BOLIVAR ROADS
SOUTH JETTY
CAUSEWAY
GALVESTON
GULF OF MEXICO
WEST BAY
GALVESTON ISLAND
SCALE
0
5 N.M.
SAN LUIS PASS

Fig. 7.72 The Galveston Bay System

point for the development of mathematical water quality models for the Galveston Bay System (Espey et al. 1968). Mathematical models for water quality parameters developed or under development for the Galveston Bay Project include both steady-state and time-varying models. The time-varying models are employed to represent long-term (i.e., tidal-averaged) variations as well as intratidal variations which are of particular importance in considering the local effects of individual outfalls. Due to the shallowness of the Bay and hence the augmented mixing effects of waves, Galveston Bay is nearly vertically homogeneous, except, of course, in the ship channels and in the neighborhood of large discharges. Therefore the distribution of parameters is represented by vertically averaged models, i.e. with two horizontal spatial dimensions. The Houston Ship Channel above Morgan Point is represented as a one-dimensional system for detailed studies of the transport and reactions of polluting substances in this area.

A time-varying two-dimensional hydrodynamic model is used to calculate the current velocities, which are retained on magnetic tape and used as basic input, appropriately time-averaged, for the advection terms in the various water quality models. Parameters for which extensive model development and verification have been undertaken are salinity, temperature, BOD and DO. However, application to other parameters such as coliforms, nutrients and a toxicity parameter is an important adjunct to this work. Computational techniques used in the time-varying and steady-state water quality models are straightforward: in the former, explicit time-differencing is employed, and in the latter, the concentration field is determined by successive overrelaxation using the finite-difference approximation to the steady-state mass balance equation.

The Galveston Bay Project activities include an extensive data collection program which is subdivided as follows:

1. a large-scale sampling program involving monthly sampling of the entire bay system;

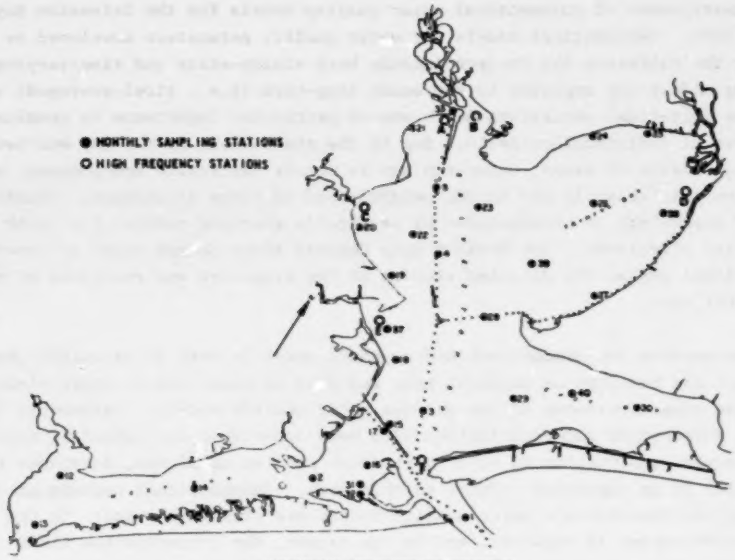
2. a high-frequency sampling program in which numerous samples are collected at short-time intervals over a tidal cycle at selected points in the bay.

The large-scale program maintains thirty-nine sampling locations throughout the Bay and Ship Channel as shown in Figure 7.73. Samples are taken at two points in the vertical at each station in the bay proper, and Ship Channel stations are sampled at four locations in the vertical. All are sampled within roughly a twelve-hour period. Water quality parameters measured in this data program include dissolved oxygen, temperature, pH, conductivity, chlorinity, BOD, total and fecal coliform, nitrogen series and total phosphates. The high-frequency program has concentrated on evaluating the short-term variations of certain water quality parameters including dissolved oxygen, conductivity, temperature, pH, and some data on free CO_2. Some limited current measurements and meteorological observations are made during both the large-scale and the high-frequency programs.

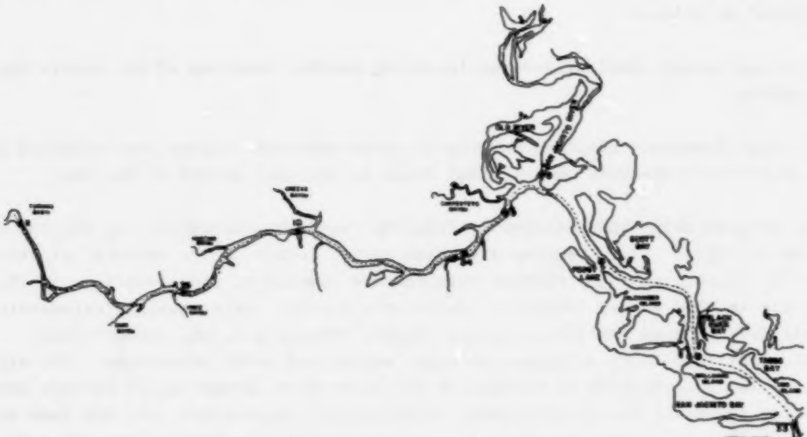
5.1.1 Hydrodynamic Model

5.1.1.1 Model Formulation and Application

The hydrodynamic model for Galveston Bay is based principally upon the work of Reid and Bodine (1968), which is a numerical solution to the equations of motion appropriately simplified for the computation of storm surges in Galveston Bay. The model represents


● MONTHLY SAMPLING STATIONS
○ HIGH FREQUENCY STATIONS

GALVESTON BAY SAMPLING STATIONS


SAN JACINTO BAY
GALVESTON BAY

HOUSTON SHIP CHANNEL SAMPLING STATIONS

Fig. 7.73 Galveston Bay Project sampling stations.

the Bay system in two horizontal spatial dimensions, and employs the time-dependent vertically integrated equations of motion and continuity, allowing for rainfall, wind stress, and bottom friction, but neglecting transport of momentum and the Coriolis force. Allowances are made in this model for submerged barrier reefs and the overflow of low-lying barrier islands. The dynamic equations of motion and of continuity are written

$$\frac{\partial U}{\partial t} + gD\frac{\partial H}{\partial x} = X - fQUD^{-2}$$

$$\frac{\partial V}{\partial t} + gD\frac{\partial H}{\partial y} = Y - fQVD^{-2}$$

and
$$\frac{\partial H}{\partial t} + \frac{\partial U}{\partial x} + \frac{\partial V}{\partial y} = R$$

where U, V = vertically integrated x and y components of velocity (dimensions L^2/T)

H = water level elevation relative to MSL

D = water depth

Q = $\sqrt{U^2+V^2}$, the magnitude of the vertically integrated velocity

f = nondimensional bottom coefficient of friction

R = rainfall rate

X, Y = the x, y components of wind stress divided by the water density

The wind stress is represented by

$X = KW^2 \cos \theta$

$Y = KW^2 \sin \theta$

in which W = wind speed

θ = angle between the wind velocity vector and the x axis

K = an empirical function of wind speed, proportional to the drag coefficient (see, e.g., Wu 1969)

The numerical solution to these equations is accomplished by representing the Galveston Bay area by a two-dimensional lattice with a constant grid spacing and solving the finite-difference form of the equations by advancing the solution explicitly through finite time increments over the entire grid system. The storm surge predictions of Reid and Bodine (1968) were obtained using a grid spacing of two nautical miles. A depth and frictional coefficient are assigned to each of the nodes. The parameter values for each node represent averages over the area represented by that particular cell. With each node is also associated the necessary information to determine that cell's orientation with respect to surrounding land barriers and internal boundary constraints. A set of initial condition and boundary conditions is required including, among other factors, tidal stage at the passes, freshwater inflow, and topography. The initial conditions used in the model also affect the duration and behavior of the starting transients.

The storm surge model (Reid and Bodine 1968) was calibrated by adjusting the frictional coefficient f to reproduce measured tides at selected points in Galveston Bay. The friction factor was varied between 0.01 and 0.001; the resulting tides are shown in Figure 7.74 for Kemah Docks and the railroad causeway. It can be seen that if the bottom friction factor is too large, the surge wave amplitudes are reduced, and the higher harmonics are filtered out of the tidal oscillations. For a friction factor too small, the computed amplitudes of the tidal waves are too large. The friction factor that was finally selected was a constant 0.0025 throughout the bay. Shown in Figure 7.75 are the final computed tides compared with the observed tides at Morgan Point, South Texas City Dike and the South Jetty.

Although the storm surge model is probably inadequate for the computation of currents under less singular conditions, it was thought to form a suitable point-of-departure for the development of a more general model to be used in the Galveston Bay Project. The equations of motion were augmented by inclusion of the Coriolis deflection and the nonlinear field accelerations (when important, as in the locality of large discharges, see Section 5.1.3). The bottom stress expressions were reformulated in terms of Manning's n . A grid spacing of one nautical mile proved to be the best compromise between spatial refinement and constraints of computer time. The initial verification of the GBP one-nautical-mile model consisted of comparison of predicted tidal variations with recorded tidal elevations. The model was operated using the driving tide displayed in Figure 7.76 along with comparisons between measured and computed tides for various points in the Galveston Bay system. In general, good agreement was obtained. It should be noted that a slight transient is in evidence during the first one-and-a-half tidal cycles (i.e., the measured and computed tides are slightly out of phase), but by the third cycle reasonable phase correlation is obtained.

The primary output of the hydrodynamic model is a time history of the velocity pattern over the bay, which is required for the advection terms of the water quality models. As an example of the velocity information provided by the hydrodynamic model, calculations have been made using the input tide of Figure 7.76 and the ten-year average freshwater inflows to the bay given in Table 7.15. For use in the steady-state mass conservation model, the results of the hydrodynamic model were time-averaged over a tidal cycle to remove the oscillatory components of tidal period and thus providing the "net" nontidal velocities. The results are displayed in Figure 7.77 as a vector pattern of the net velocities superimposed on a map of the system. The outline of the boundary of the model grid structure is also displayed. As an example of the use of the model to predict the effects on currents resulting from physiographic modifications, the model was operated using identical input conditions with the addition of a proposed diversion of 3,200 cfs across Umbrella Point. The model results in Figure 7.78 depict the alteration in the net flow pattern as a result of the diversion.

5.1.1.2 Comparison of Mathematical Hydrodynamic Model with Physical Model

In April 1969, experiments were performed in the Ship Channel physical model (see Section 5.2) at Vicksburg as a part of the GBP. The mathematical model was operated using the input tide and freshwater inflow as specified in the physical model test, and velocities obtained from the mathematical model were compared to those measured in the physical model. The comparisons were made for three ranges in the bay, namely (1) one station between Atkinson Island and Mesquite Knoll, (2) two stations between Red Fish Island and Smith Point, and (3) two stations between Red Fish Island and Eagle Point (Ranges 1 and 6 in Figure 7.92). Current velocities measured in the physical model were reported to the nearest 0.1 ft/sec at hourly intervals during the tidal cycle. Time histories of velocity from the mathematical model calculations

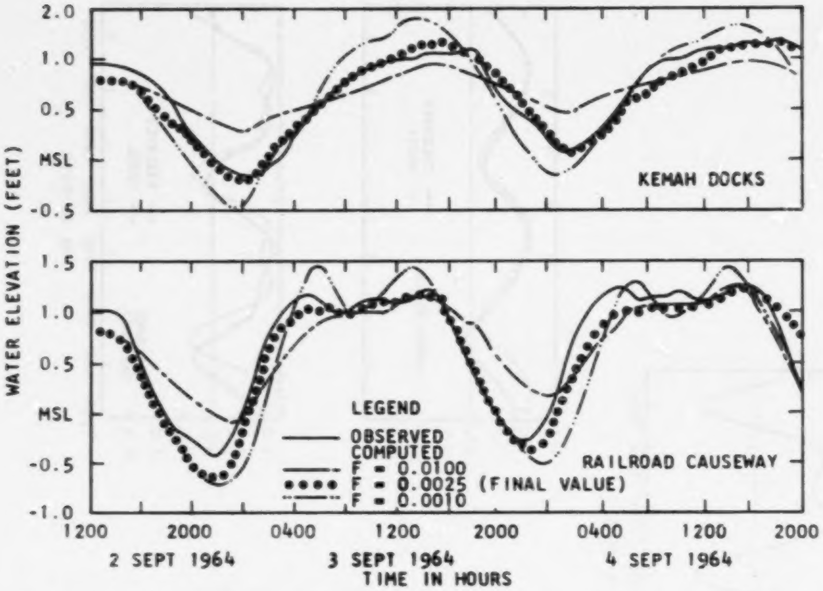


Fig. 7.74 Computed Astronomical Tide for two locations in Galveston Bay for three different friction factors: Observed value also shown. After Reid and Bodine (1968).

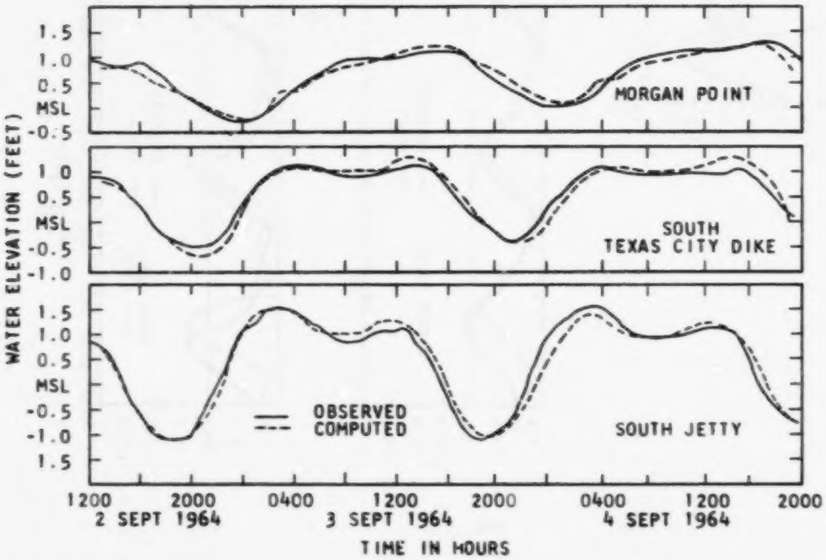


Fig. 7.75 Comparison of observed and computed Astronomical Tide for three locations in Galveston Bay using final friction factor. After Reid and Bodine (1968).

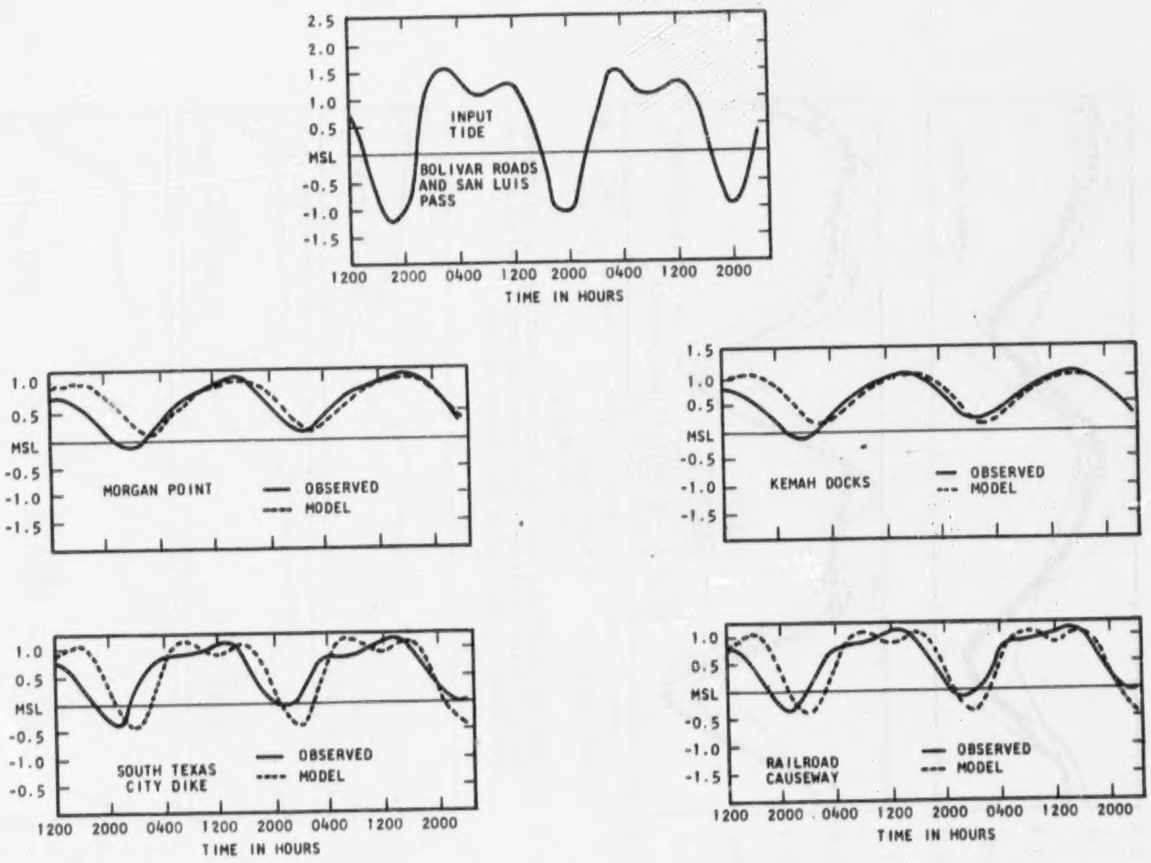


Fig. 7.76 Comparison of measured and computed tidal elevations in Galveston Bay (Stover et al. 1971).

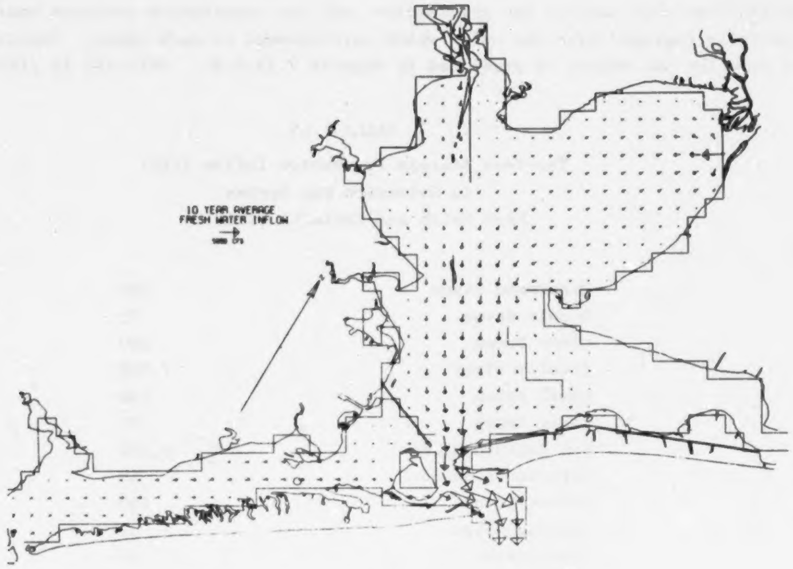

10 YEAR AVERAGE
FRESH WATER INFLOW

Fig. 7.77 Calculated tidal-averaged velocities for ten-year-mean inflow.

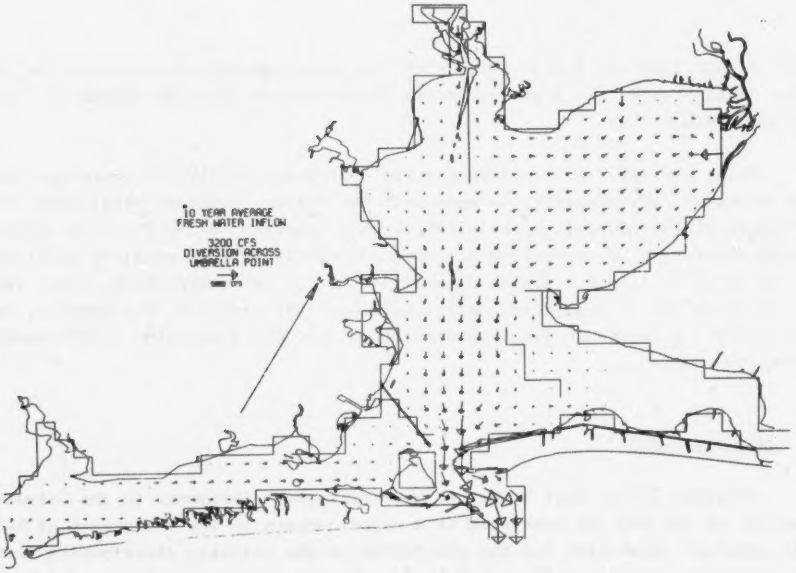

10 YEAR AVERAGE
FRESH WATER INFLOW
3200 CFS
DIVERSION ACROSS
UMBRELLA POINT

Fig. 7.78 Calculated velocities for conditions of Fig. 7.77 with added diversion across Umbrella Point (top right).

were obtained at each node in the grid system, and for comparative purposes these model results were spatially averaged over the cells which corresponded to each range. Comparison of the results from the two models is presented in Figures 7.79-7.81. Velocity is plotted as a function of time over one tidal cycle, with the positive ordinate representing flood. With the exception of high water slack period on the range between Red Fish Island to Eagle Point, the results compare quite well.

TABLE 7.15

Ten-Year Average Freshwater Inflow (cfs)
to Galveston Bay System
From Smith and Kaminski (1965).

Dickinson Bayou	100
Double Bayou	75
Clear Creek	200
Trinity River	7,900
Cedar Bayou	150
Goose Creek	25
San Jacinto River	2,100
Carpenters Bayou	18
Greens Bayou	150
Hunting Bayou	35
Vince Bayou	15
Sims Bayou	90
Brays Bayou	125
Buffalo Bayou	340
Total Inflow	11,323

Point currents in the Galveston Bay System are highly influenced by the local effects of wind, waves and physiography, so even with the correct boundary conditions, comparison of the mathematical hydrodynamic model with currents measured in the field is difficult. For this reason the above type of comparison of computed velocities with physical model measurments is of some value as it allows a degree of verification of the hydrodynamic model velocities independent of their use in the water quality models. This provides, for example, some protection from incorporating errors in velocity prediction into the dispersion coefficients used in the water quality models.

5.1.2 Salinity Model

Salinity is the most important hydrobiological parameter in the Galveston Bay estuary. Preservation of the natural ecosystem is a major concern to the management of Galveston Bay, and this requires capability for the prediction of the salinity distribution in the Bay, particularly with regard to effects of the decrease in freshwater inflow due to urban consumption and upstream diversion, e.g., the Texas Water Plan (Texas Water Development Board 1968).

Figure 7.82 displays a typical summer salinity distribution in Galveston Bay. The marked influence of the Houston Ship Channel on the isohalines should be noted. As stated previously, the predominant sources of inflow into Galveston Bay are the San Jacinto River -

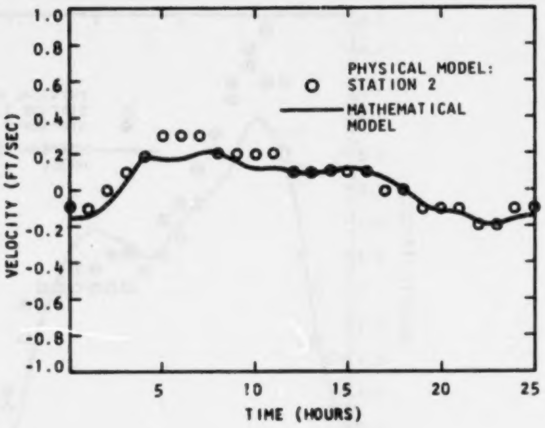


Fig. 7.79 Comparison of velocities from physical model and mathematical model. Range 1, Atkinson Island to Mesquite Knoll (see Fig. 7.92).

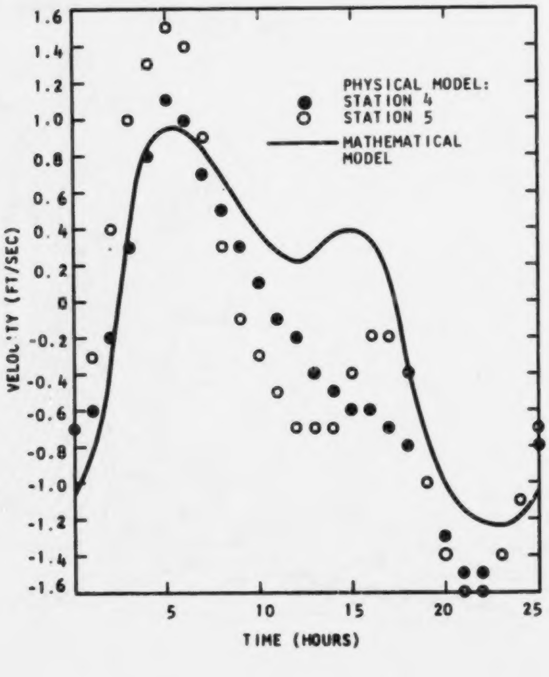


Fig. 7.80 Comparison of velocities from physical model and mathematical model. Range 6, Red Fish Island to Eagle Point (see Fig. 7.92).

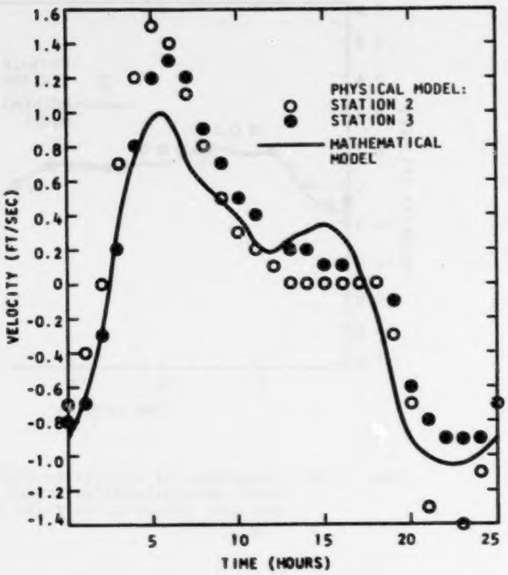


Fig. 7.81 Comparison of velocities from physical model and mathematical model. Range 6, Red Fish Island to Smith Point (see Fig. 7.92).

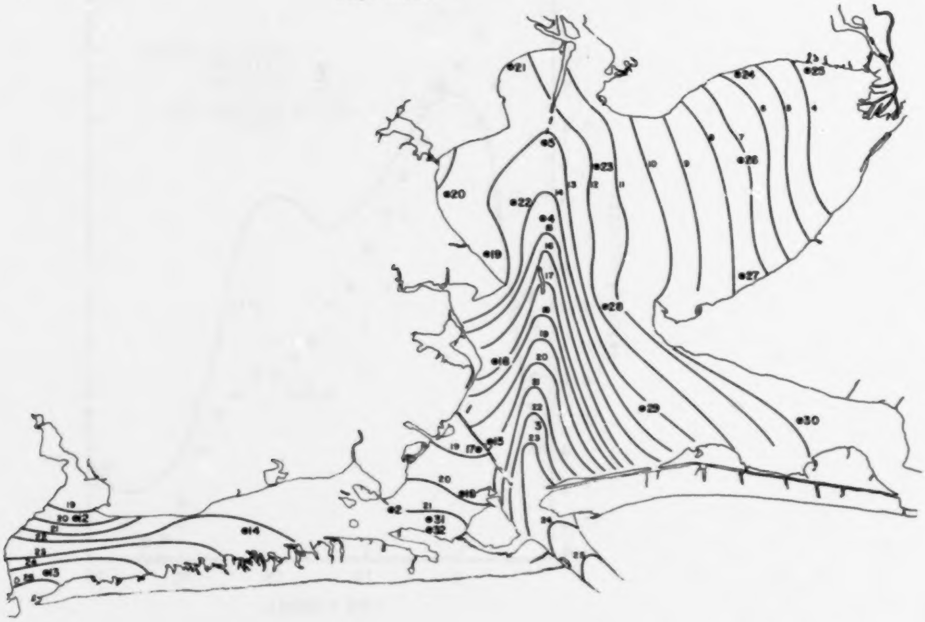

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Fig. 7.82 Salinity contours from measurements of 17 September 1968 in Galveston Bay.

Houston Ship Channel and the Trinity River (although the lesser tributaries discharging into Galveston Bay are occasionally significant). These inflows tend to be highly erratic, as is indicated in Figure 7.83. Variations in inflow of two orders of magnitude within a month span are not uncommon. Due to the irregularity of these inflows, as well as wind conditions, evaporation and tidal currents, the salinity at a given point in the bay tends to fluctuate markedly over a wide range. Evaluation of the model operation has been difficult because of this natural fluctuation in the measured data together with the lack of precise input information (e.g., complete inflow records, evaporation measurements, and records of saline discharges in the Bay). Most of the verification to date has been directed toward the "steady-state" calculations. Steady-state distributions appear to be acquired in the Bay when the inflows are sustained for several months (which usually occurs at low flows). Moreover, the effects of even large fluctuations in the inflows can be removed by time-averaging over sufficiently long periods so that quasi-equilibrium profiles are obtained.

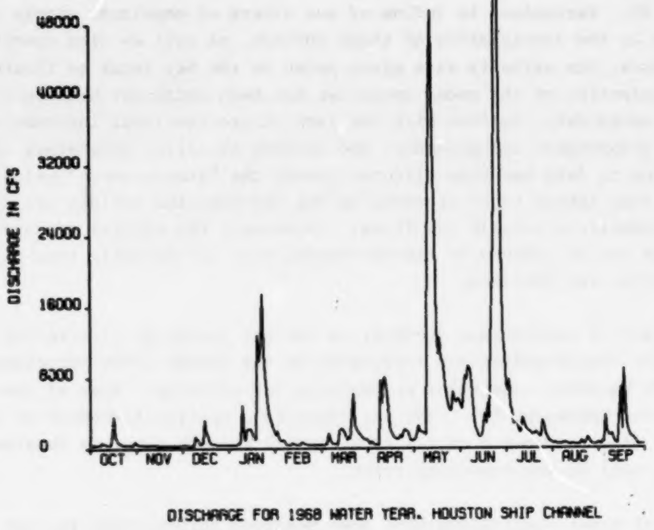
The calculation of equilibrium profiles in the Bay system is effected by successive overrelaxation using the finite-difference expression of the steady-state two-dimensional mass transport equation with boundary conditions appropriate for salinity. Most of the work performed on salinity in the Galveston Bay Study has employed a spatial increment of one nautical mile. The net current (i.e., averaged over a tidal cycle) at each point is obtained from the hydrodynamic model and used in the advective terms.

Comparisons of model predictions with mean measured chlorinities for two different "averaging times" are given in Tables 7.16 and 7.17. The empirical chlorinities of Table 7.16 are the means over the three-month period November 1968 through January 1969. During this period the inflow was generally quite low but with intermittent peaks ranging to as much as 13,000 cfs in the Ship Channel. The model velocities were obtained assuming relatively low inflows of 230 cfs in the Ship Channel and 550 cfs in the Trinity. Agreement between model predictions and the averaged field data is satisfactory with the exception of Stations 24 and 25 in Upper Trinity Bay. These stations, however, are near a low, marshy area, where they are subject to random overland runoff from the Trinity. Table 7.17 tabulates the predicted concentrations using the ten-year mean inflows of Table 7.15. For comparison, the average of a year of monthly salinity measurments (July 1968 through June 1969) are given. Dispersion coefficients were the same for both computations and were obtained from measurements of chlorinity made in the summer of 1968.

5.1.3 Thermal Discharge Model

As a part of the Galveston Bay Project and with the joint support of Houston Lighting & Power Co. (Houston), Central Power & Light Co. (Corpus Christi), and Gulf States Utilities Co. (Beaumont), an intensive study was performed of the behavior and distribution of temperature in selected estuaries of the Texas coast. A principal objective of this study was the development of a model for predicting the temperature profile in the vicinity (viz. within the "intermediate" or "transitional" mixing region, see Chapter IV) of the thermal discharges into shallow areas. The basis of this model is the time-dependent vertically integrated expression of the conservation of energy, employing formulations of the various heat fluxes through the surface (Stover et al. 1971). As with the other mathematical models developed by the Galveston Bay Project, the solution is accomplished by finite-difference techniques, in this case using explicit time-differencing for stepping the solution forward in time.

For application to the immediate vicinity of an outfall, both the temperature model and the associated hydrodynamic model were implemented using a (horizontal) spatial grid of relatively fine resolution, i.e., with a spatial increment of a few hundred feet. Boundary



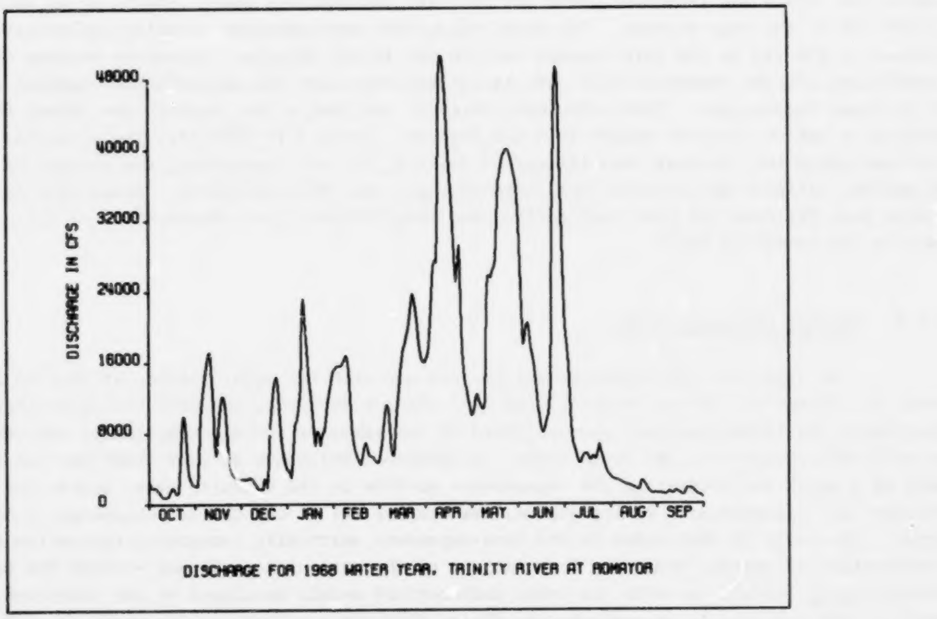


Fig. 7.83 **Inflows in Trinity River and Houston Ship Channel (at Morgan Point) for 1968 water year.**

TABLE 7.16

Comparison of Steady-State Model Predictions and Measured (Nov. 1968 - Jan. 1969 Average) Chlorinities (ppt)

GBP Station	Predicted	Measured	GBP Station	Predicted	Measured
1	17.0	14.6	18	12.3	11.3
2	15.0	13.1	19	10.5	10.3
3	13.4	13.2	20	9.6	9.8
4	10.6	12.1	21	10.1	10.0
5	10.2	11.8	22	10.4	9.9
6	10.0	10.4	23	8.7	7.9
7	10.0	9.2	24	7.3	3.8
8	7.1	6.4	25	6.7	3.0
9	9.1	8.8	26	7.5	7.2
10	8.4	8.2	27	7.9	7.2
11	7.2	7.2	28	10.1	7.8
12	12.5	13.3	29	11.4	9.4
13	15.4	15.0	30	10.8	8.5
14	14.4	12.8	31	15.4	14.9
15	13.5	13.0	32	15.3	14.5
16	15.3	14.6	33	10.0	11.4
17	15.4	14.0	34	9.0	8.9
			35	7.9	7.8

TABLE 7.17

Comparison of Steady-State Model Predictions and Measured (July 1968 - June 1969 Average) Chlorinities (ppt)

GBP Station	Predicted	Measured	GBP Station	Predicted	Measured
1	15.3	14.6	18	8.0	8.7
2	13.3	11.5	19	5.9	6.3
3	9.5	12.4	20	5.2	5.8
4	5.9	9.6	21	5.4	6.7
5	5.5	8.7	22	5.7	6.7
6	5.3	6.4	23	3.6	5.2
7	5.3	5.8	24	2.4	2.8
8	2.2	3.4	25	1.9	2.0
9	4.3	5.3	26	2.5	3.6
10	3.7	4.9	27	2.8	3.4
11	2.9	3.8	28	4.9	5.0
12	11.8	10.3	29	6.2	6.6
13	14.6	13.7	30	5.6	5.8
14	13.1	11.4	31	13.5	12.6
15	9.5	10.6	32	13.4	12.6
16	13.4	11.8	33	5.3	7.9
17	13.4	11.9	34	4.2	5.7
			35	3.3	4.5

conditions for the hydrodynamic model were obtained by interpolation from the results of the coarse, one-nautical mile grid hydrodynamic model described in Section 5.1.1. The momentum equations used in this hydrodynamic model are the same as those of Section 5.1.1 with the addition of the nonlinear field acceleration terms, as in such proximity to the outfall these terms become significant. Buoyancy effects are neglected.

This model was applied to several steam power plant discharges along the Texas coast. One such application is to the Houston Lighting & Power Company P. H. Robinson Generating Station which is located on the western shore of Galveston Bay and discharges into upper Galveston Bay in water of nominally five foot depth. The plant has a maximum generating capacity of 1,475 megawatts and utilizes 667,000 gallons per minute (approximately 1,500 cfs) of once-through cooling water with a 17.6°F rise across the condensers. The outfall area is shown in Figure 7.84. The outfall structure consists of low weir, boat barrier, and a pair of parallel sheet-metal groins extending out about 1,000 feet perpendicular to the shore. The computational grid system for both the hydrodynamic and temperature models as applied to the outfall site is based on a 500 by 500 foot lattice covering an area of approximately seven square miles near the discharge. The grid spacing provides a fairly fine representation of the physical system, including the shoreline, groins and variations in the depth. The orientation of the grid was dictated by the groins and shoreline, as these features required precise representation within the computational framework.

As an example of the thermal discharge model operation, a comparison is made between some of the field data obtained at the P. H. Robinson site and the associated model results. The data were collected during the period 2-3 October 1969. Water temperature surveys were performed by traversing the plume while towing multiple-depth temperature sensors. The outputs of the sensors were continuously recorded on a chart recorder inside the boat. On-site meteorological data were also collected (displayed in Figure 7.85), and the plant operating conditions were obtained. The tidal range was larger than normal, so that tidal currents were more pronounced than usual. The general direction of the wind was from the shore and the plume was only slightly affected as it was sheltered from the wind by bluffs along the shoreline. Later in this period, however, the wind shifted and the movement of the plume became dominated by wind-driven currents. Water temperature surveys were made at approximately 2:00 p.m., 5:00 p.m., and midnight on 2 October, and at 9:00 a.m. and noon on 3 October. In Figure 7.86 are shown temperature contour plots obtained from the model at times corresponding to the water temperature surveys, with the boat traverses and recorded temperatures superimposed upon the predicted contours. The disagreement between the model predictions and the measured temperatures was greater than expected for the midnight survey; it was suggested to be due to difficulties in determining positions at night (Stover et al. 1971). The computer time required for these computations, using a time step of three minutes, was approximately four minutes per tidal cycle on the UNIVAC 1108 computer, including the time required for generating the temperature contour plots.

Another example of the operation of the thermal discharge model, but not in Galveston Bay, is an application to the Central Power and Light Company Nueces Bay Generating Station, which is located on the south shore of Nueces Bay. Nueces Bay, a small secondary embayment off Corpus Christi Bay, has a surface area of approximately 20,000 acres and an average water depth of approximately three feet. It receives limited freshwater inflow from the Nueces River during most of the year. The Nueces Bay plant has a maximum generating capacity of 240 megawatts and utilizes 120,000 gallons per minute (270 cfs) of once-through cooling water which is pumped from the Corpus Christi Ship Channel at a depth of thirty feet and is discharged into Nueces Bay from a dredged channel. The plant imparts a 15°F temperature rise across the condensers.

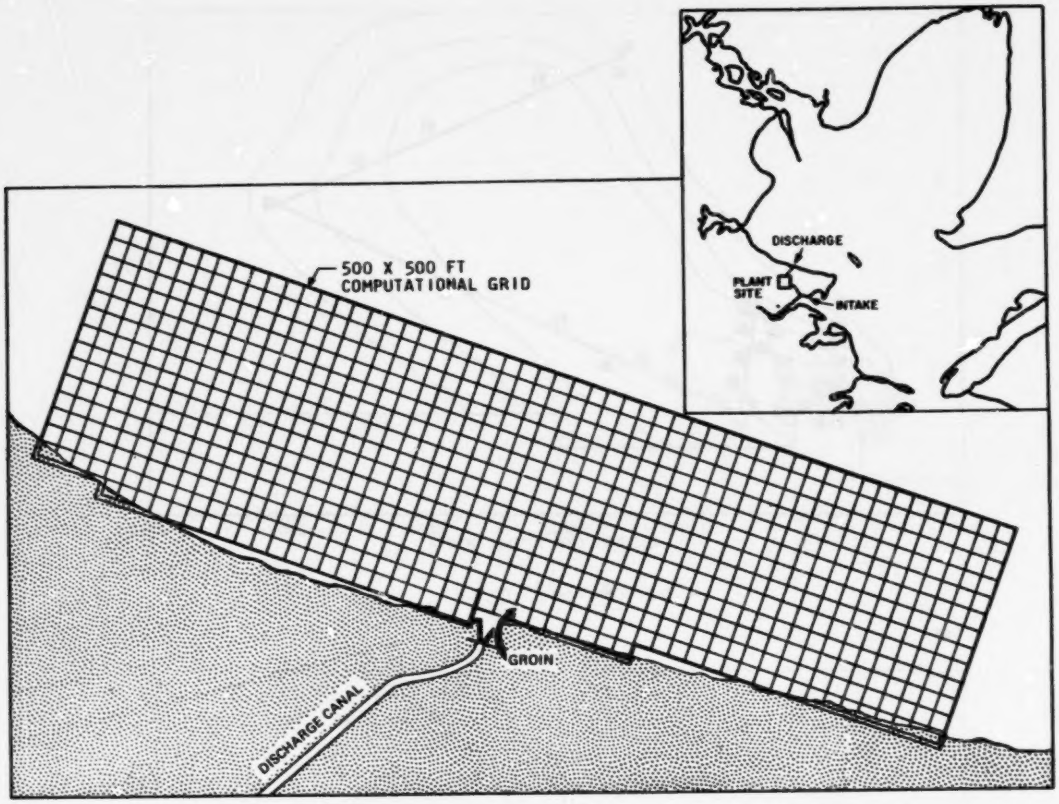

500 X 500 FT
COMPUTATIONAL GRID
DISCHARGE
PLANT SITE
INTAKE
GROIN
DISCHARGE CANAL

Fig. 7.84 Location map and computational grid for thermal discharge model.

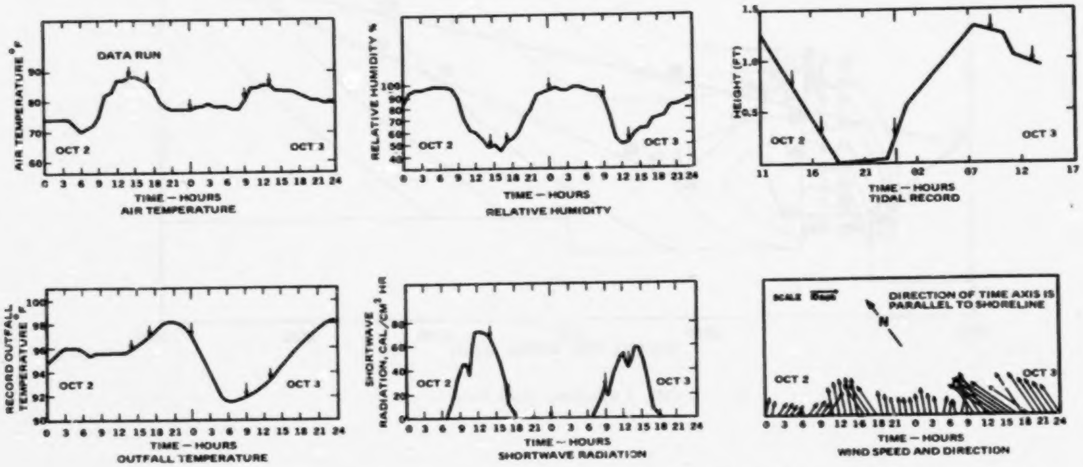
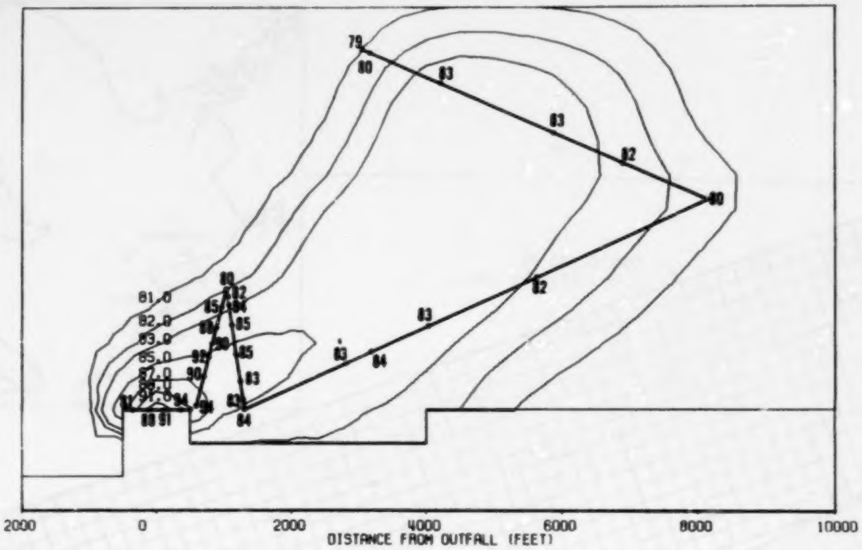
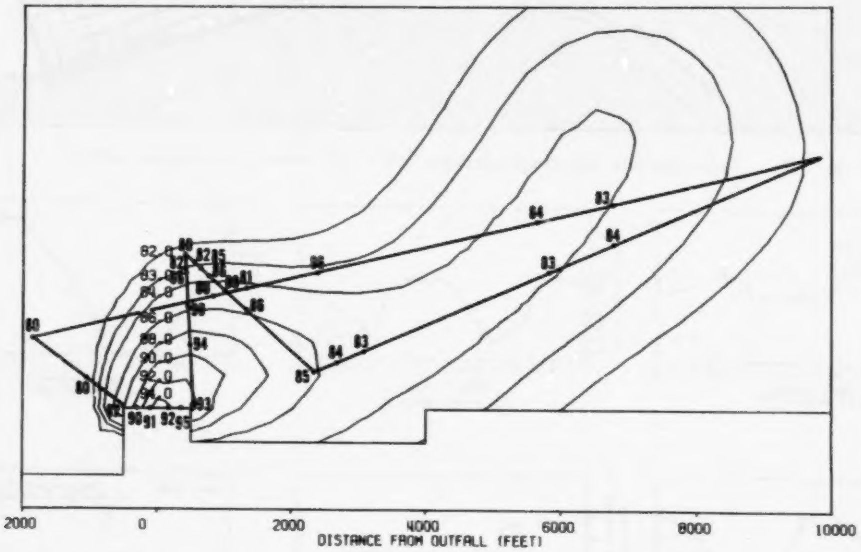


Fig. 7.85 Environmental conditions at P. H. Robinson Plant on 2 - 3 October.

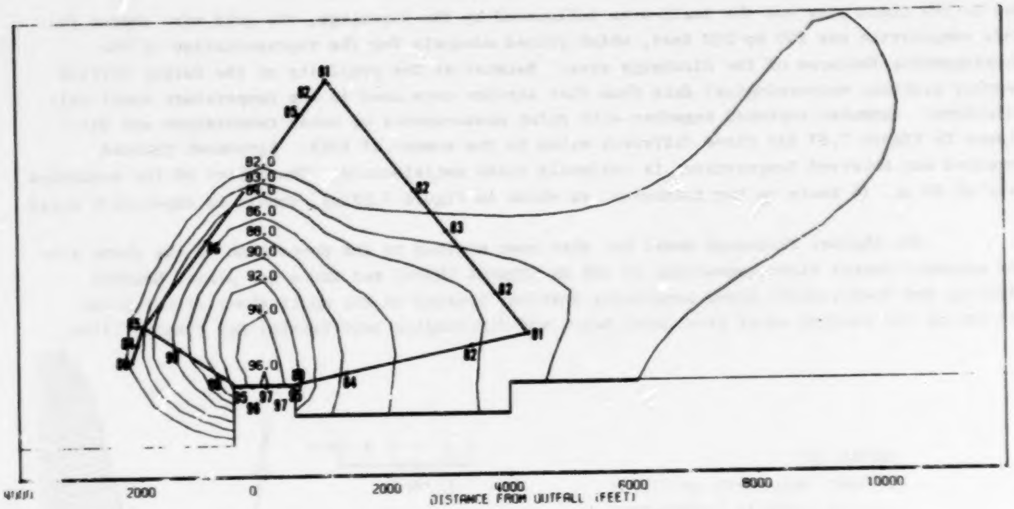


(a) 2 October, 2:00 P.M.

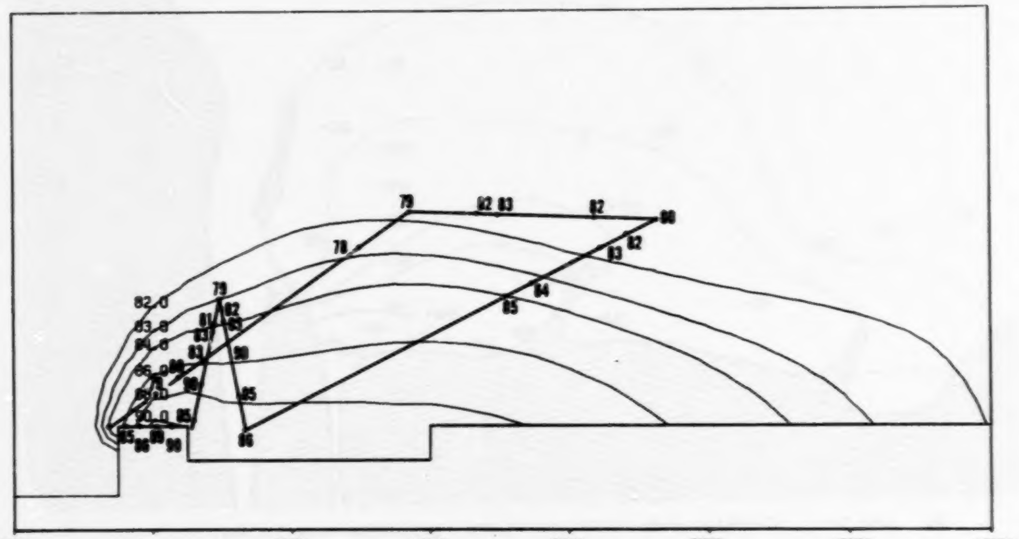


(b) 2 October, 5:00 P.M.

Fig. 7.86 Calculated temperature (^{O}F) contours with measurements from boat traverses. P. H. Robinson discharge in Galveston Bay. From Stover et al. (1970).



(c) 2 October, Midnight.

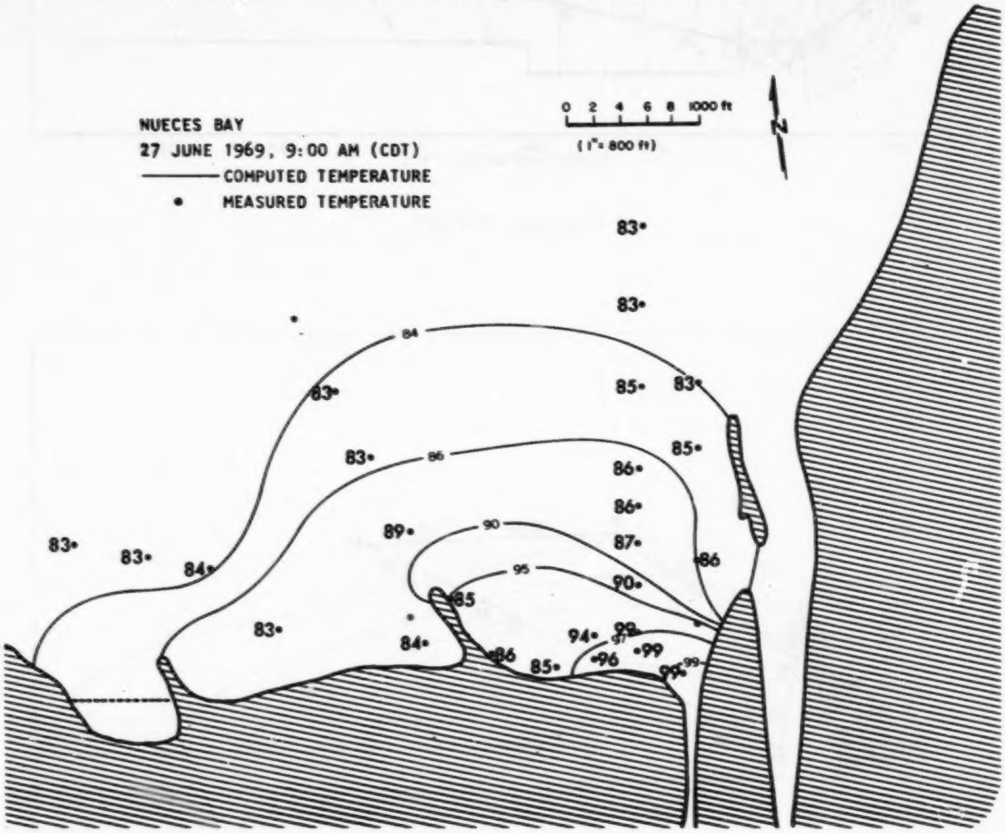


(d) 3 October, 9:00 A.M.

Fig. 7.86 Continued.

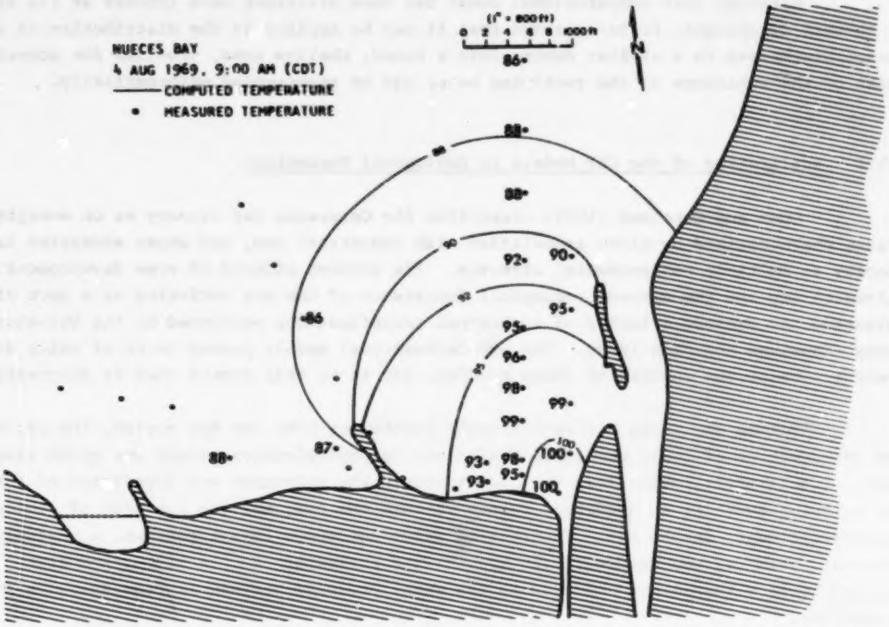
Due to the plant size and the small area influenced by the discharge, the grid size chosen for this computation was 200 by 200 feet, which proved adequate for the represzentation of the physiographic features of the discharge area. Because of the proximity of the Corpus Christi weather station, meteorological data from that station were used in the temperature model calculations. Computed contours together with point measurements of water temperature are displayed in Figure 7.87 for three different dates in the summer of 1969. Agreement between computed and observed temperatures is evidently quite satisfactory. The effect of the southeast wind of 10 ca. 15 knots on the isotherms, as shown in Figure 7.87(a), should be expecially noted.

The thermal discharge model has also been applied to the prediction of the plume size for expanded Nueces Plant operations of 569 MW (TRACOR 1970a) and for a new plant, Houston Lighting and Powers Cedar Bayou Generating Station, located on the north shore of Galveston Bay taking its cooling water from Cedar Bayou and discharging into Trinity Bay (TRACOR 1970b).

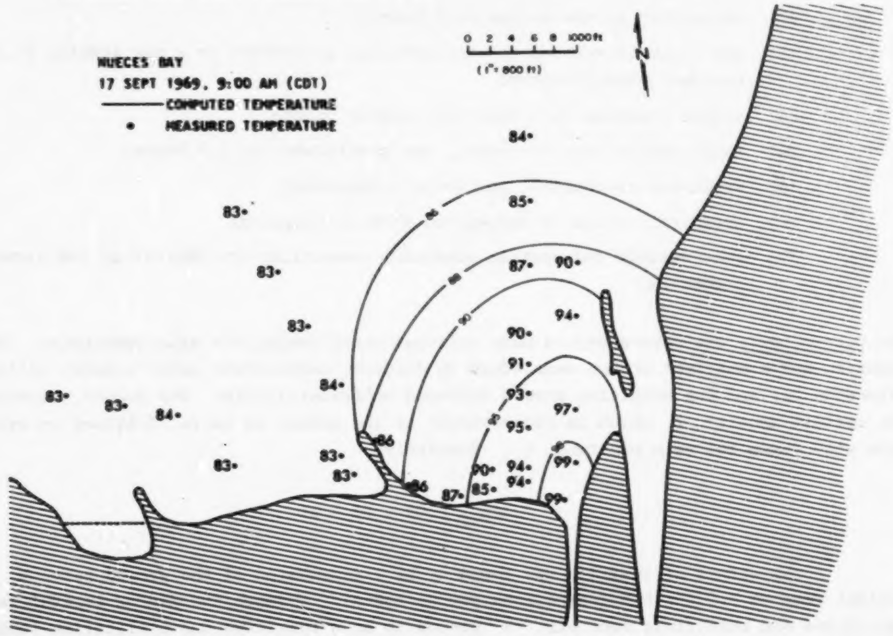

NUECES BAY
27 JUNE 1969, 9:00 AM (CDT)
COMPUTED TEMPERATURE
MEASURED TEMPERATURE
0 2 4 6 8 1000 ft
(1" = 800 ft)
N
83
83
84
83
85
83
83
86
85
86
86
89
90
87
83
83
84
86
95
90
85
83
84
86
85
94
99
97
96
99
99
99

(a) JUNE DATA, SOUTHEAST WIND AVERAGING 15 MPH, DISCHARGE FLOW 270 cfs

Fig. 7.87 Comparison of calculated temperatures from thermal discharge model and measured temperatures for three environmental conditions.


NUECES BAY
4 AUG 1969, 9:00 AM (CDT)
COMPUTED TEMPERATURE
MEASURED TEMPERATURE
(1" = 800 ft)
0 2 4 6 8 1000 ft
N
86
88
88
90
92
90
95
86
95
96
98
99
99
100
88
87
93
98
100
93
95
100

(b) AUGUST DATA CALM, DISCHARGE FLOW 270 cfs


NUECES BAY
17 SEPT 1969, 9:00 AM (CDT)
COMPUTED TEMPERATURE
MEASURED TEMPERATURE
0 2 4 6 8 1000 ft
(1" = 800 ft)
N
84
83
85
83
87
90
83
94
90
91
84
83
83
84
93
97
95
83
83
90
94
99
83
86
87
85
94
99

(c) SEPTEMBER DATA, CALM, DISCHARGE FLOW 270 cfs

Fig. 7.87 Continued

Although this computational model has been discussed only insofar as its application to thermal discharges, it is apparent that it may be applied to the distribution of any substance discharged in a similar manner into a broad, shallow area, provided the sources and sinks of the substance in the receiving water can be represented mathematically.

5.1.4 Application of the GBP Models to Ecological Parameters

Odum and Copeland (1969) classified the Galveston Bay estuary as an emerging new system characterized by close association with Industrial Man, and whose ecosystem is subjected thereby to multiple environmental stresses. The evident effects of area development on Galveston Bay and the extreme ecological importance of the Bay motivated as a part of the Galveston Bay Project a series of biological investigations performed by the University of Texas (Copeland and Fruh 1970). The GBP mathematical models proved to be of value in interpreting some of the results of these studies, and it is this aspect that is discussed here.

Due to the large and varied waste discharges into the Bay system, the possibility of the introduction of toxic compounds inhibitory to phytoplankton growth was given careful attention. Specifically, objectives were to ascertain the existence and importance of toxicity, the relative toxicity at different points through the Bay, and the toxicity of variously treated effluents in the Bay. In order to carry out these investigations, a phytoplankton bioassay parameter was devised: the growth-rate parameter k . A blue-green alga (Coccochloris elebans) was selected as the assay organism because it possesses the following properties:

(1) ubiquitous to the marine environment;

(2) was shown to respond to environmental parameters in a way similar to the resident phytoplankton;

(3) stable organism that does not readily mutate;

(4) rapid growth rate of roughly one generation per 2.5 hours;

(5) sensitive to nutrient and toxic components;

(6) ordinarily stays in suspension with no clumping;

(7) considerable information available concerning its physiology and growth potential.

The Coccochloris was maintained in pure cultures until needed for experimentation. The test organism and a nutrient medium were added to diluted, pasteurized water samples collected in Galveston Bay and the resulting growth followed colorimetrically. The growth, represented by the optical density D which is proportional to the number of cells, followed an exponential form with (base 10) rate constant k . Precisely,

$$\log_{10} (100 \times D) = kt$$

The effect of toxicity was found to be a depression of the growth rate k from the optimal rate of 2.0 (or 6.6 generations per 24 hours). Through the use of careful laboratory procedures and sufficient controls, k proved to be a sensitive and utilitarian indicator of the toxicity of the sample water. The following comments from Copeland and Fruh (1970) amplify the interpretation of the k parameter.

> To assess the effects of toxicity on the test organism, its growth rate is measured in liquid culture tubes. This growth rate is expressed as a k value (the increase of log optical density x 100 per 24 hours). . . . In this manner, an average k can be obtained for a growth curve; thus giving a realistic growth evaluation. Any lags in growth or erratic growth will be incorporated in this calculation.
>
> In order to put the k values in perspective with growth rates and productivity, we endeavor to discuss the meaning of the k value. This will allow us to interpret the full meaning of k and how it relates to the evaluation of toxicity in the natural setting.
>
> k is the slope of a line on a graph and is defined as the log of the change in optical density during a 24-hour period. This simply represents the ability of the cells to reproduce--or the number of generations of the test organism per 24-hour period. . . . A k of 0.301 represents one generation per day (or a doubling of the original number of cells in the test culture) and a k of 1.9 represents 6.3 generations per day (or a doubling of the cells in the original culture 6.3 times). This means that the k value in relation to the number of generations is linear and that a doubling of k means a doubling of growth rate.
>
> Optical density is used as the measurement criteria and a change in optical density of 0.1 means a change in the number of cells of approximately 1.05 x 10^7 cells per ml. . . . To relate optical density changes, cells numbers and k values, consider the change in optical density from 0.1 to 1.0 in 24 hours. This represents a k value of 1.0 (change in log of 0.1 to log of 1.0 is equal to a k of 1) and a change in the number of cells per ml from 1.05 x 10^7 to 10.5 x 10^7--or a doubling of the cell population 3.3 times (thus relating k and optical density in terms of growth of the population).

Values of k were obtained for six stations in the Bay system from February through December 1969. These six stations were Trinity River, Houston Ship Channel, Bolivar Roads, Dickinson Bay, Hannah's Reef, and the Texas City Dike. Experimental model computations were made to predict the distribution of k through the Bay system assuming a steady-state distribution. The period August through October represented a sustained low inflow period and appeared to approximate an equilibrium state. It was assumed that k was a conservative parameter transported by advection and diffusion through the Bay, with the important boundaries being the Trinity River, Houston Ship Channel at Morgan Point, and Bolivar Roads. Thus the solution technique employed was the same as the steady-state salinity calculations of Section 5.1.2 (i.e., successive overrelaxation on the finite-difference approximation of the mass conservation equation) with boundary conditions appropriate for toxicity. Dispersion coefficients were the same as employed in the salinity work. Model predictions were compared with the measured k values for the period August through October. To eliminate the effect of experimental fluctuations the measured data was averaged for the period August-October, and the averaged values for the boundary points were used in the model computations. Additional model calculations were made averaging the data over the periods March-October and July-October but the agreement between predicted and observed k values was somewhat poorer; this is attributed to the transient effects of large freshwater inflows during spring. The inflows, boundary conditions, and comparisons of model results with measured values of k are presented in Tables 7.18, 7.19 and 7.20, respectively. The agreement between measured k and model predictions is quite satisfactory.

Copeland and Fruh (1970) also investigated the relation of the phytoplankton toxicity parameter k to the species diversity indices of various populations. Species diversity was estimated by

$$H = \sum_i \frac{n_i}{N} \log \frac{n_i}{N}$$

where n_i is the number (or weight) of individuals in the i th species and N is the total number (or weight) of individuals in the collection. Species diversity indices were determined

TABLE 7.18

Inflows for Computations of Steady-State k Distribution

River or Tributary	Inflow (cfs)
Trinity River	564
Houston Ship Channel (at Morgan Point)	230
Clear Creek	126
Dickinson Bayou	110
Double Bayou	78
Cedar Bayou	44
Goose Creek	40

TABLE 7.19

Averaged k Used for Boundary Conditions

Boundary	Averaging Period		
	August-October	July-October	March-October
Houston Ship Channel	0.99	1.06	1.08
Trinity River	0.49	0.54	0.76
Bolivar Roads	1.98	1.91	1.91

TABLE 7.20

Computed and Observed (mean) k Values for Galveston Bay Stations

Station	Averaging Period					
	August-October		July-October		March-October	
	pred.	obs.	pred.	obs.	pred.	obs.
Dickinson Bay	1.34	1.45	1.33	1.35	1.33	1.51
Hannah's Reef	1.21	1.35	1.20	1.47	1.20	1.40
Texas City Dike	1.66	1.70	1.65	1.61	1.65	1.59

for finfish (by number and by weight), nekton, zooplankton, benthos and phytoplankton from seasonal samples at each of the GBP stations (Figure 7.73) over a year. The model calculations of the distribution of k in the Bay system were compared with the mean annual diversity indices observed in the system. Quite good correlation was obtained between the phytoplankton diversity and the growth parameter, as is evident in Figure 7.88. A degree of correlation might be expected *a priori* between empirical measurements as both parameters are a measure of the response of the phytoplankton community to the presence of inhibitory constituents, in which case the correlation between measured diversity and a predicted k constitutes an additional degree of verification that k can be modeled as a transported parameter. More importantly however, this correlation attests to the possibility of using models as predictors of the ecological "health" of the Bay. An example of the correlation between the predicted k and another population diversity is shown in Figure 7.89. Correlation between nekton weight diversity and predicted k values is somewhat poorer, but this is not especially surprising

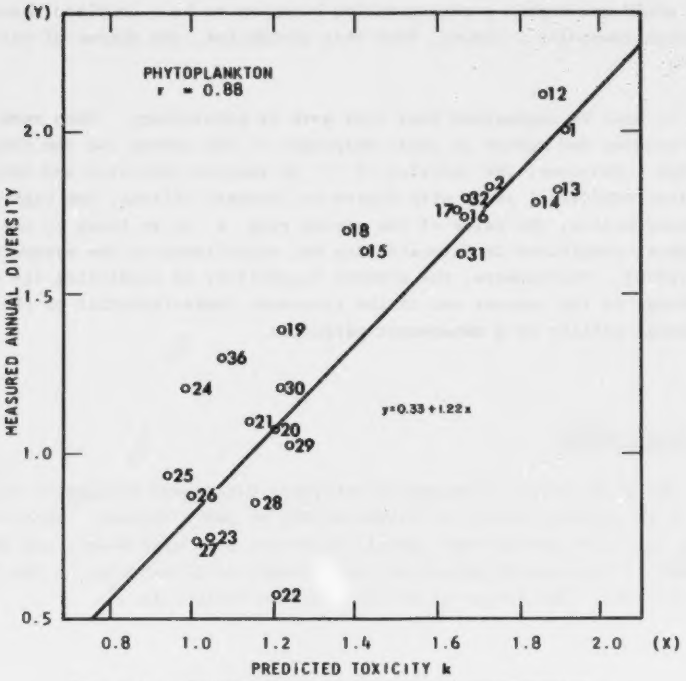


Fig. 7.88 Relationship between annual mean species diversity and model predictions of toxicity parameter (Copeland and Fruh 1970). Numbers are GBS sampling stations, Fig. 7.73.

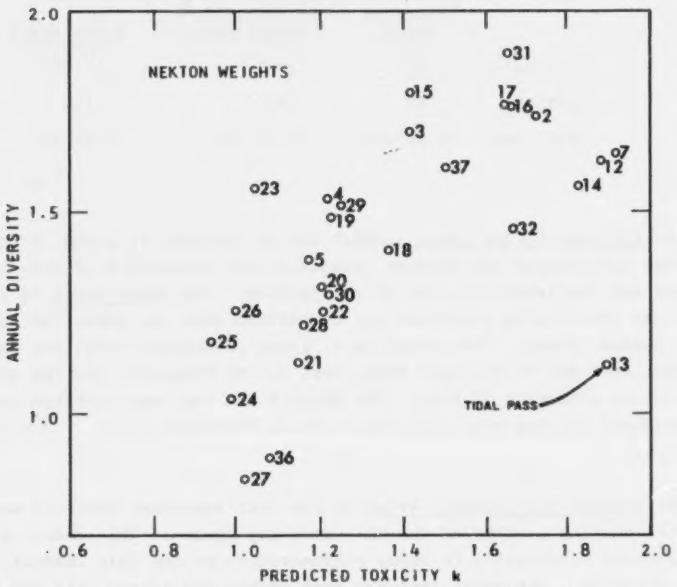


Fig. 7.89 Relationship between predicted k and annual mean nekton weight diversity. Copeland and Fruh (1970).

since one would not expect a phytoplankton bioassay to be a complete measure of the response of the nekton community. Indeed, from this standpoint, the degree of correlation obtained is encouraging.

It must be emphasized that this work is preliminary. Much remains to be learned about the sources and nature of toxic materials in the system and the dynamic behavior of their distribution. Moreover, the relation of k to species diversity and other ecological indicators requires additional study with regard to seasonal effects, the higher trophic levels, and so on. Nevertheless, the value of the growth rate k as an index to toxic substances and to the ecological conditions in Galveston Bay was established by the extensive work of Copeland and Fruh (1970). Furthermore, the evident feasibility of predicting its spatial distribution from knowledge of its sources and of the transport characteristics of the system indicates that it may possess utility as a management parameter.

5.2 PHYSICAL MODELS

The U. S. Corps of Engineers Waterways Experiment Station at Vicksburg, Mississippi, operates three physical models of Galveston Bay or parts thereof. These three models are designated Galveston Bay Entrance Model, Galveston Bay Surge Model, and the Houston Ship Channel Model. The spatial extent of these models is illustrated in the location maps, Figures 7.90-7.92. The scale ratios are given in Table 7.21.

TABLE 7.21

Scale Ratios in Galveston Bay Physical Models

	Entrance Model	Houston Ship Channel Model	Surge Model
Horizontal	1:500	1:600	1:3,000
Vertical	1:100	1:60	1:100
Tidal Day	29.91 min.	19.25 min.	4.97 min.

The Entrance Channel Model, which can be operated as either a fixed-bed or a moveable-bed model, was constructed for studies related to the relocation of the entrance channel to Galveston Bay and the rehabilitation of the jetties. The Surge Model is a highly distorted model which was constructed primarily for comparison with the numerical surge model developed by Reid and Bodine (1968). This model is a "gross phenomena" model and includes all of Galveston Bay, East Bay to Rollover Pass, West Bay to Freeport, and the entire surrounding flood plain up to elevation 20 feet. The Surge Model has been verified for water surface elevations throughout the Bay with data from a known hurricane surge. (Hurricane Carla was used for this purpose.)

The Houston Ship Channel Model is the most important physical model from the standpoint of water quality studies of the Galveston Bay system. This model is a very large fixed-bed model designed principally to study sedimentation in the Ship Channel, and related maintenance dredging. The model includes most of the Bay system, all the Houston Ship Channel to above the Turning Basin, the important freshwater inflows and the most significant physiographic features throughout the Bay. The model does not include West Bay, but rather is terminated on the west near the Galveston Causeway. Similarly, only a portion of East Bay is included. The Ship Channel portion of this model has been verified with tidal amplitude, salinity, and velocity data collected within the Channel during selected portions of a one-year period. Verification within the shallower parts of the Bay proper has not been as thoroughly carried out.

The Alpha and Gamma barriers (Figure 7.92) have been proposed to protect the developed areas of the Bay from hurricane surge. They are provided with wide navigation gates that are to be kept open in normal circumstances but closed to form a solid barrier whenever a hurricane threatens. Concern has been expressed that the presence of the barriers, even when open, may reduce the exchange of Bay waters with the Gulf so as to alter salinity profiles and to reduce the assimilative capacity and hence the general quality of the system. The Ship Channel model has been employed to study the distribution of contaminants (using dye releases) and the

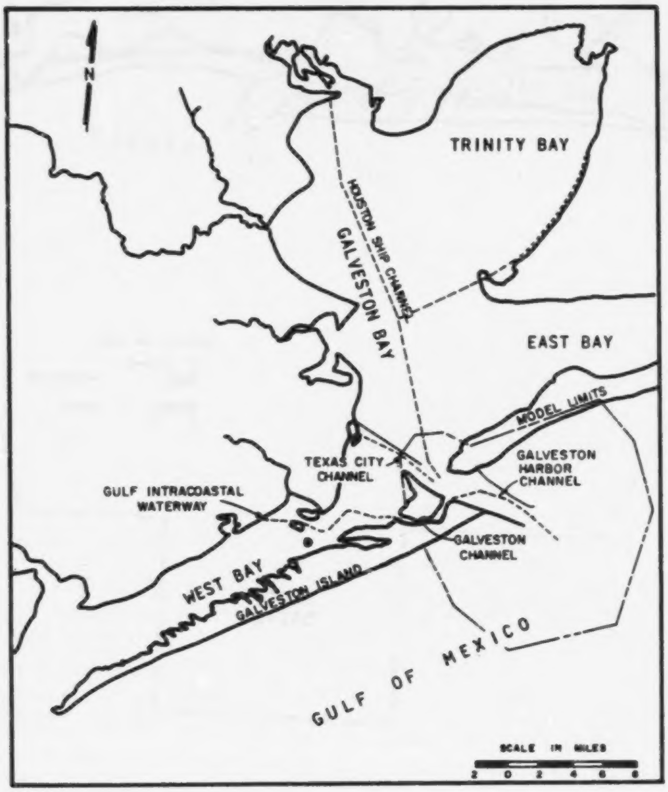
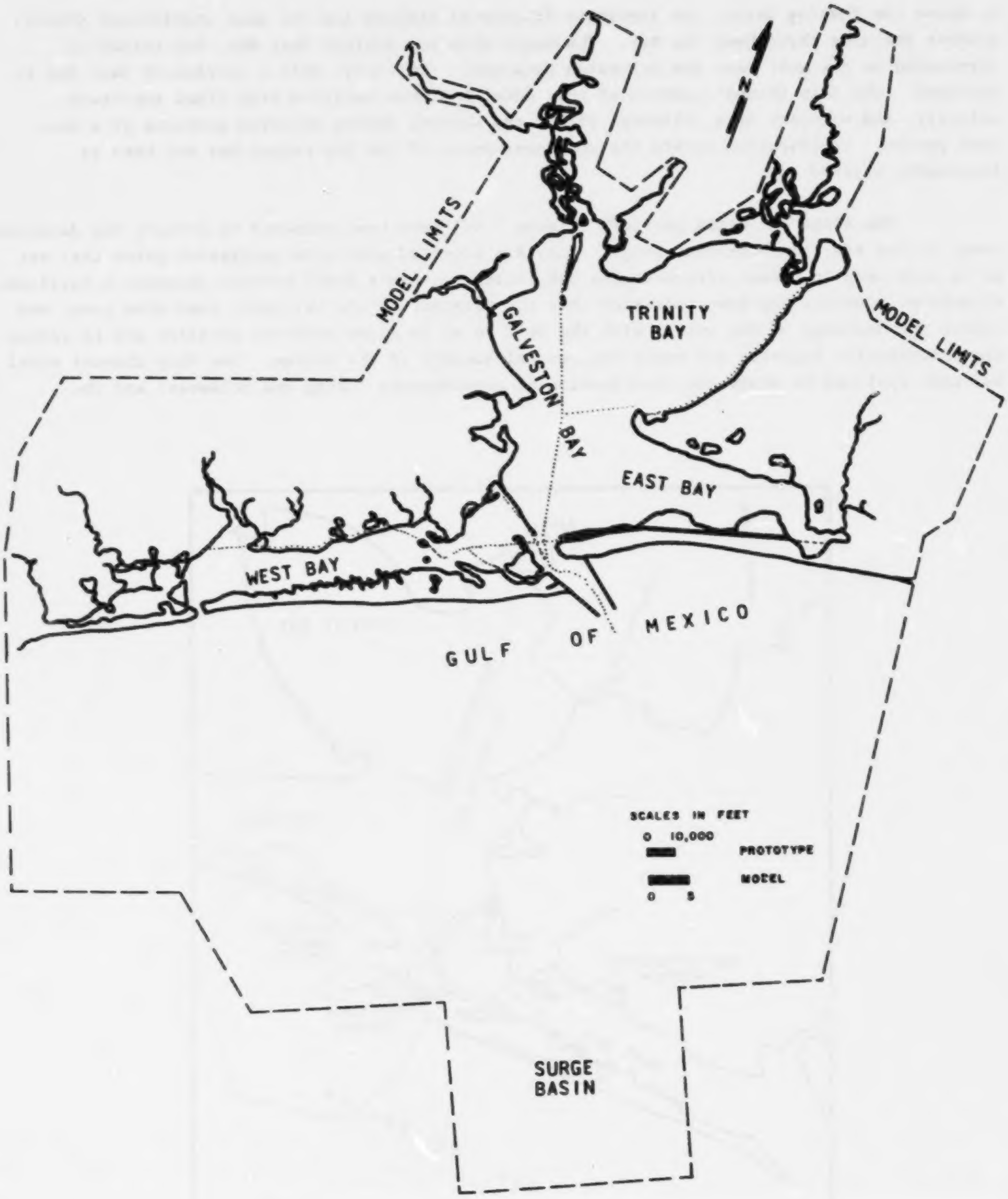

N
TRINITY BAY
HOUSTON SHIP CHANNEL
GALVESTON BAY
EAST BAY
MODEL LIMITS
GALVESTON HARBOR CHANNEL
TEXAS CITY CHANNEL
GULF INTRACOASTAL WATERWAY
GALVESTON CHANNEL
WEST BAY
GALVESTON ISLAND
GULF OF MEXICO
SCALE IN MILES
2 0 2 4 6 8

Fig. 7.90 Entrance Channel Model--Waterways Experiment Station.


MODEL LIMITS
N
TRINITY BAY
MODEL LIMITS
GALVESTON BAY
EAST BAY
WEST BAY
GULF OF MEXICO
SCALES IN FEET
0 10,000
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MODEL
0 5
SURGE BASIN

Fig. 7.91 Surge Model--Waterways Experiment Station.

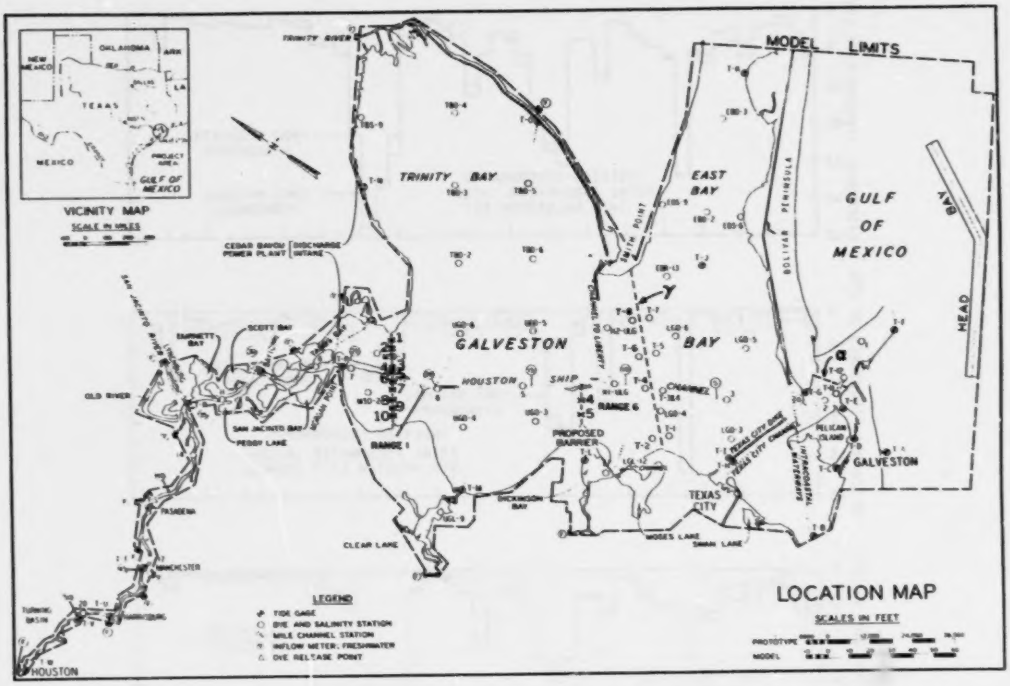
VICINITY MAP
SCALE IN MILES
OKLAHOMA
ARK
NEW MEXICO
TEXAS
LA
MEXICO
PROJECT AREA
GULF OF MEXICO
TRINITY RIVER
MODEL LIMITS
TRINITY BAY
EAST BAY
GULF OF MEXICO
BOLIVAR PENINSULA
HEAD
BAY
CEDAR BAYOU POWER PLANT
DISCHARGE
INTAKE
SAN JACINTO RIVER
SCOTT BAY
BURNETT BAY
OLD RIVER
SAN JACINTO BAY
PEGGY LAKE
GALVESTON
BAY
HOUSTON
SHIP
CHANNEL
RANGE 1
RANGE 6
PROPOSED BARRIER
CHANNEL TO LIBERTY
SMITH POINT
Y
α
TEXAS CITY DIKE
TEXAS CITY CHANNEL
INTRACOASTAL WATERWAY
PELICAN ISLAND
GALVESTON
TEXAS CITY
DICKINSON BAY
CLEAR LAKE
MOSES LAKE
SWAN LAKE
PASADENA
MANCHESTER
HARRISBURG
TURNING BASIN
HOUSTON
LEGEND
TIDE GAGE
DYE AND SALINITY STATION
MILE CHANNEL STATION
INFLOW METER; FRESHWATER
DYE RELEASE POINT
LOCATION MAP
SCALES IN FEET
PROTOTYPE
MODEL

Fig. 7.92 Ship channel model (Waterways Experiment Station) showing proposed Gamma and Alpha hurricane barriers.

salinity distribution in the Bay with and without the proposed hurricane barriers. It has also been used to study the influence on currents and salinity patterns of natural and regulated inflows and the proposed Cedar Bayou Plant diversion across Umbrella Point. Some documentation of this work has appeared (Bobb and Boland 1970) and the remainder is presently in preparation. The results of the model operation will be briefly discussed, insofar as salinity is concerned, in this section.

Two sets of inflows were used in the model tests (Figure 7.93), the natural hydrograph for 1965 and the same hydrograph with projected 1980 regulation and a 3,200 cfs diversion across Umbrella Point. Additional boundary inputs employed for the model studies were the input tide shown in Figure 7.94 and a Gulf salinity of 32.5 ppt. This input tide is the average prototype tide at Pleasure Pier which was determined from several years record.

The effects of flow regulation alone on salinities as predicted by the model are illustrated in Figure 7.95 which are annual time histories at various stations. Station

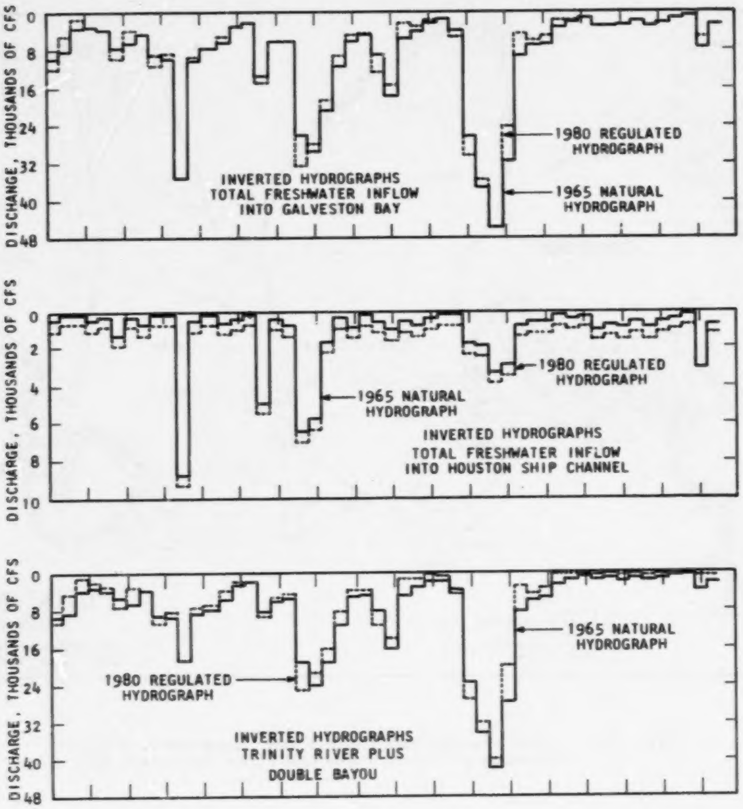

Fig. 7.93 Inflow conditions--Galveston Bay Physical Model.

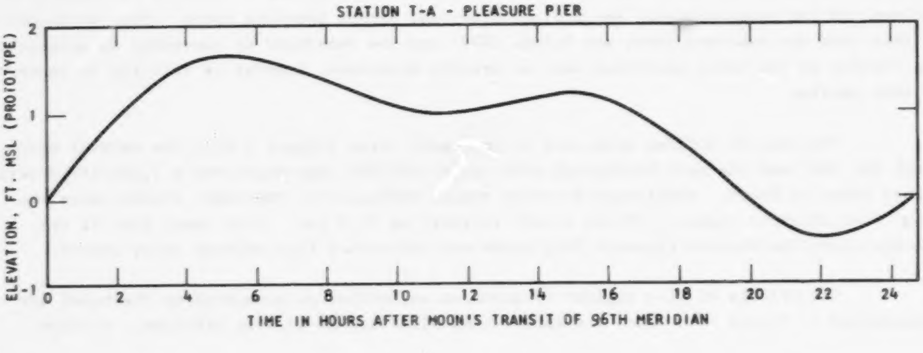

Fig. 7.94 Input tide at Bolivar Roads used in physical model experiments.

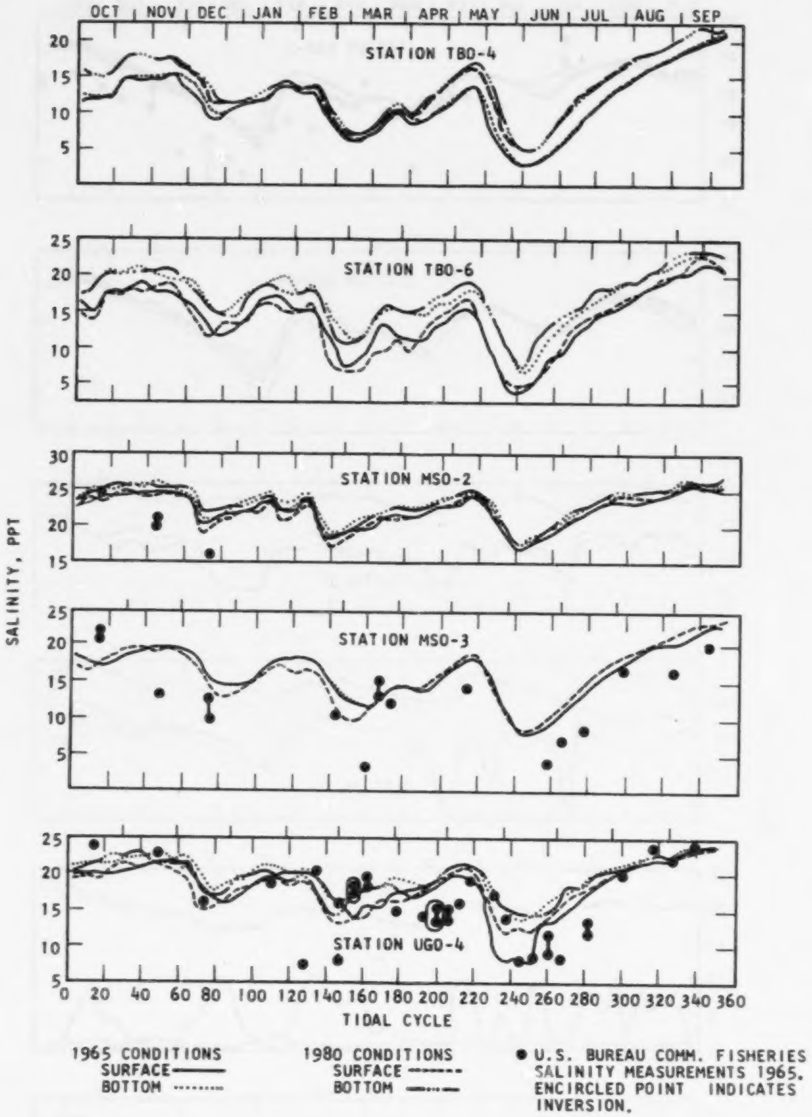

Fig. 7.95 Salinity measurements in physical model for natural conditions (1965) and regulated inflows (1980). After Bobb and Boland (1970). 1965 USBCF salinity data from Pullen and Trent (1969).

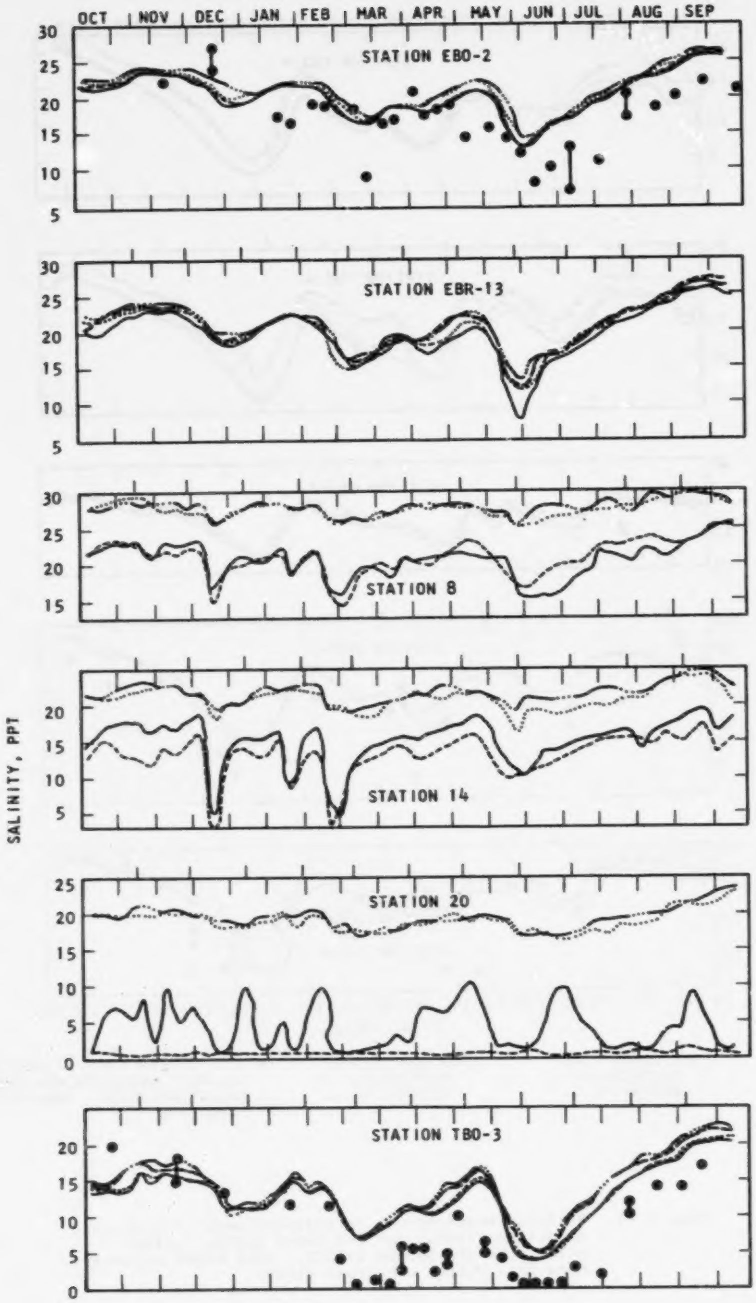

Fig. 7.95 Continued

locations are shown in Figure 7.92. The effects may be summarized as slight, being most manifest in the upper reaches of the Ship Channel.

During the 1965 water year, salinity data was collected by the Bureau of Commercial Fisheries (Galveston) throughout the Bay (Pullen and Trent 1969). A number of USBCF stations correspond to those monitored in the model and it is of interest to compare the salinity histories from the prototype with the 1965 model predictions. Accordingly, the empirical data for representative stations in Upper Galveston Bay, Trinity Bay and East Bay are plotted along with the physical model results in Figure 7.95. Both surface and bottom measurements were obtained but in most cases the difference did not exceed .5 o/oo. When a larger surface-to-bottom difference existed, both measurements are plotted. (At Station UGO-4, the circled points indicate a salinity inversion.) It is evident that the model results generally are in poor agreement with empirical data. It is the opinion of the staff of the Waterways Experiment Station that the 1965 inflow hydrographs used for the model tests did not account for all of the freshwater inflow to the bay complex, especially to Trinity Bay during the February-March period. They note that this same problem has been encountered with other estuary models, and in every case where the inflow hydrographs have been refined to the point of accounting for all of the freshwater inflow, what first appeared to be a discrepancy between model and prototype salinities was resolved. They did not recommend such a refinement in the case of the Galveston Bay barrier studies, since the results desired from the model were the changes in salinity caused by the barriers, rather than the absolute salinities with barriers installed for specific inflow conditions (Simmons 1970).

The effects of the planned Alpha and Gamma hurricane barriers on salinity were determined for the 1980 flow conditions. Examples of these model results are given in Figures 7.96 and 7.97, respectively. The effect of either barrier appears from these results to be slight compared to the natural fluctuation in salinity throughout the Bay.

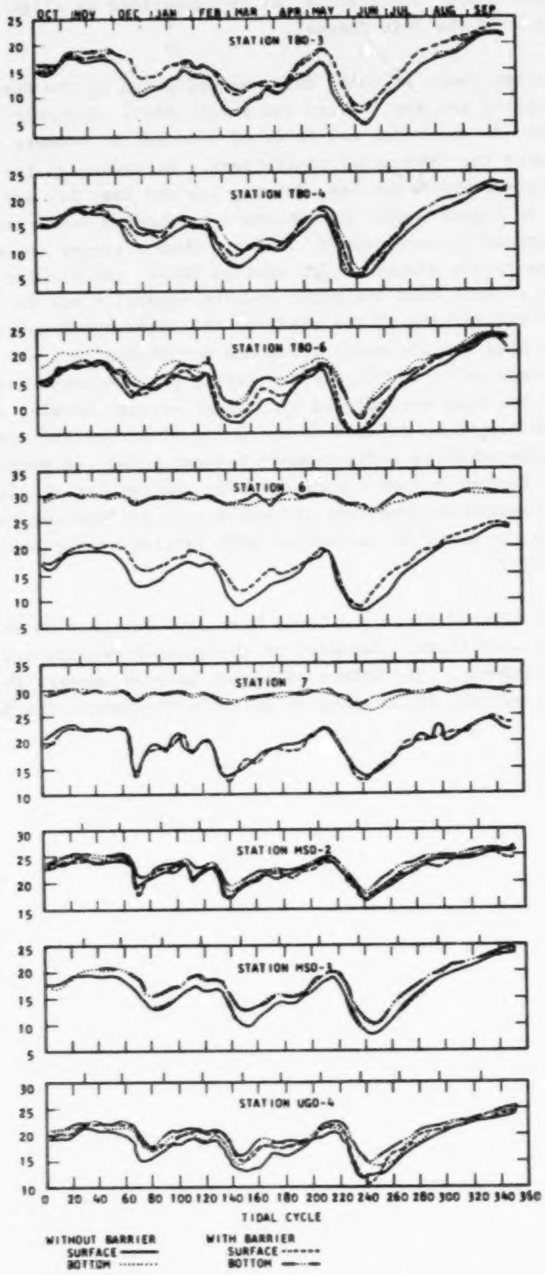

Fig. 7.96 Salinity measurements from physical model for 1980 inflows, showing effects of Alpha Barrier. After Bobb and Boland (1970).

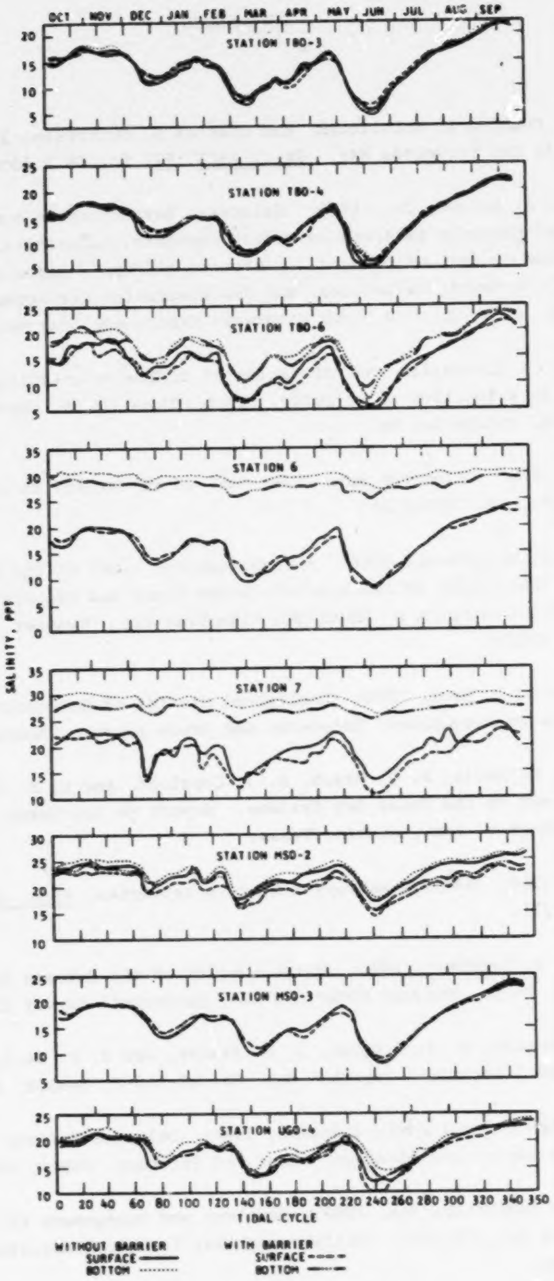

Fig. 7.97 Salinity measurements from physical model for 1980 inflows, showing effects of Gamma Barrier. After Bobb and Boland (1970).

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CHAPTER VIII

BIOLOGICAL MODELING IN ESTUARIES: A NOTE

G. J. Paulik

The preceding material in this report documents considerable progress in modeling the dynamic behavior of physical and chemical parameters in estuaries. In this section we examine the feasibility of extending these numerical modeling techniques to simulate the ecological processes which are so important in determining man's commercial, recreational and aesthetic use of estuaries.

1. CHARACTERISTICS OF ANIMAL COMMUNITIES IN ESTUARIES

Fish and birds are the most visible members of the animal communities associated with estuaries and have received the most attention from both the general public and the management agencies. Few nations of the world have major marine fisheries so closely associated with a system of estuaries as does the United States. About two-thirds of the economic value of the commercial catch and most of the marine sport catch is composed of species which spend at least part of their lives in estuaries (McHugh 1966). Except for the tuna fleet, the United States has no true high-seas distant-water fishing fleets.

Estuaries play a variety of critical roles in the life histories of important species of fish and shellfish. Some sessile animals are permanent residents of the estuaries, while the anadromous species pass through the estuaries during migrations to freshwater spawning, rearing and maturing areas. Other species use the estuaries as spawning and rearing areas. Table 8.1 (from McHugh 1966) lists commercially exploited species which are estuarine-dependent. Four of the top five commercial species by value (shrimp, salmon, tuna, oysters and menhaden) landed by the U. S. flag fleet are closely associated with estuaries. The role of the estuarine environment in the life history of each of these four species is described below in order of species importance.

Penaeid shrimp breed in the sea at varying distances from land. A series of early life history stages, nauplii, protozoea and mysis, are completed as the larval shrimp move from the sea toward the estuary. The estuarial stage of life begins about three to five weeks after hatching and lasts from two to four months. The juvenile shrimp then return to sea where they are recruited into the fishery and complete their life cycle.

Salmon deposit their eggs in the gravel of freshwater streams, rivers or lakes with upwelling areas. After hatching, the young fry may spend anywhere from a few weeks to several years in fresh water. The downstream migrants, either as fry or as smolt, pass through the estuaries where they often linger for extended periods of time. High biological productivity

TABLE 8.1

ESTUARINE-DEPENDENT SPECIES TAKEN IN UNITED STATES FISHERIES (After McHugh 1966)

Common Names	Scientific Names
Alewives	*Alosa pseudoharengus*, *A. aestivalis*
Catfish	*Ictalurus* spp.
Croaker	*Micropogon undulatus*
Drums	*Pogonias cromis*, *Sciaenops ocellata*
Eel	*Anguilla rostrata*
Flounders	*Psuedopleuronectes americanus*, *Paralichthys* spp., *Platichthys stellatus*
Garfish	*Lepisosteus* spp.
Gizzard shad	*Dorosoma cepedianum*
Hickory shad	*Alosa mediocris*
Hogchoker	*Trinectes maculatus*
Menhaden	*Brevoortia* spp.
Salmon	*Oncorhynchus* spp., *Salmo salar*, *Salmo gairdneri*
Scup or porgy	*Calamus* spp., *Stenotomus* spp.
Sea bass (Atlantic)	*Centropristes striatus*
Sea robin	*Prionotus* spp.
Sea trout or weakfish	*Cynoscion* spp.
Shad	*Alosa sapidissima*
Silversides	*Menidia* spp.
Smelt	Families Atherinidae and Osmeridae
Spot	*Leiostomus xanthurus*
Striped bass	*Roccus saxatilis*
Sturgeon	*Acipenser* spp., *Scaphirhynchus platorhynchus*
Swellfish	*Sphaeroides maculatus*
Tautog	*Tautoga onitis*
Tenpounder	*Elops saurus*
White perch	*Roccus americanus*
Yellow perch	*Perca flavescens*
Crabs	*Callinectes sapidus*, *Cancer magister*, *Carcinus maenas*
Horseshoe crab	*Limulus* spp.
Shrimp	*Penaeus* spp., *Xiphopenaeus* spp.
Clams	*Cardium corbis*, *Saxidomus nuttalli*, *Protothaca staminea*, *Mercenaria mercenaria*, *Mya arenaria*
Mussels	*Mytilus* spp.
Oysters	*Crassostrea* spp., *Ostrea lurida*
Periwinkles	*Littorina* spp.
Bay scallop	*Aequipecten irradians*
Terrapin	*Malaclemys* spp.
Turtles	Various species
Bloodworms	Family Glyceridae
Sandworms	*Nereis* spp.

in estuaries promotes rapid growth of the juvenile salmon during this period. While some stocks of salmon spend their entire life in an estuary or adjacent waters, it is more common for salmon to undertake extensive ocean migrations during which they may travel several thousand miles. The adult spawners must traverse the estuaries to return to their natal streams.

Oysters are estuarine residents and oyster farming is practiced extensively in U.S. estuaries. Except for the early free-swimming stages of their life which are usually completed in two or three weeks or less, oysters are sedentary. The larval stages of the oyster are specially sensitive to estuarine water quality. Oyster biologists believe that poor water quality has already caused sharp declines in certain species of oysters. One species so affected is the native oyster Ostrea lurida in the State of Washington, which is highly susceptible to pulp mill waste matter.

Menhaden of the genus Brevoorita use the extensive estuarine systems along the Atlantic and Gulf states for nursery areas. Juvenile menhaden spend the major part of the first year of life in estuaries. Larval and juvenile menhaden generally undergo a series of metamorphoses in the estuaries. Their feeding habits change from relying heavily on zooplankton as a primary food source to direct utilization of diatoms and dinoflagellates. The relative abundance of these two types of phytoplankton varies considerably from estuary to estuary, and from season to season within a single estuary.

The foregoing indicates the extent to which estuaries are related to the recruitment process in fisheries. Conditions in an estuary can be critical in determining the abundance of entering year classes. Because of the requirements for the type of environment provided by an estuary of the early life stages of some highly mobile species, transient conditions in an estuary one year may determine commercial catches several years later, hundreds or even thousands of miles away. Long range migrations complicate greatly the use of such tools as benefit-cost functions in the economic evaluation of either enhancement or deterioration of water quality in a specific estuary. The opportunity for biological modeling is perhaps greatest for these important or "key" species since a large backlog of biological information on the details of their life histories does exist.

The biological communities in estuaries depend critically on the timing of such factors as the nutrient and salinity cycles, and their life histories are synchronized with a particular temporal sequence of a series of events. Some of these events may be biological, others physical. Hedgpeth (1966) says

> From this sequence of events in several estuaries it is obvious that analysis of a factor such as gross photosynthesis by itself cannot indicate what may really be going on in an estuary; indeed the same values for different times of the year may represent different phases of a complex system. There is obviously no shortcut to understanding an estuary; the spring and early summer diatom crop may depend on the summer dinoflagellate crop, and vice versa, and the copepods may depend on this alteration of various dominant types of phytoplankton throughout the year, while the fish may depend on the interrelations of the phytoplankton and copepods or influence the phytoplankton directly if they are herbivores, and consequently have some effect on the next cycle of phytoplankton.

The high natural productivity of estuaries is often augmented by various types of fertilizing agents introduced by man. The ultimate effect of different concentrations of nutrient material on the productivity of fish stocks is not known except in the most general sense. Existing knowledge of biological processes in estuaries is far from adequate for many trophic levels. Most of the available information is concentrated either at the level of the phytoplankton which form the base of the food chain, or at the level of top predators, such as fish or birds.

Much of the phytoplankton data is concerned with the relation between nutrients and productivity, and much of the fish data with the demographic characteristics of particular stocks. Both types of information are available for certain populations of oysters. The function and structure of intermediate links in the food chain are poorly understood. Quantitative information is almost nonexistent on such crucial factors as the basic population dynamics of herbivorous and carnivorous zooplankton in estuaries, the kinetics of estuarine bacteria, and trophic interactions involving the organisms of benthic communities. Even for such birds as ducks and geese which have been studied extensively, it is not possible to guess the population consequences of eliminating the estuarine environment.

From the biological point of view the essential characteristics of the estuarine ecosystem are:

(1) high organic productivity;

(2) extreme fluctuations in both species composition and biomass with season;

(3) animal communities adapted to, and dependent upon, the precise sequencing of events in major chemical, physical and biological cycles;

(4) complex food webs whose structure and controlling mechanisms are poorly understood;

(5) unique environmental factors essential for the spawning and rearing of juvenile stages of most of the nation's important commercial and marine sport fish; and

(6) resident animal populations dominated by benthic mollusks.

2. MATHEMATICAL MODELS OF BIOLOGICAL COMMUNITIES

Entomologists and fishery scientists have constructed the most realistic mathematical models of animal populations (Watt 1966). Generally, these models have emphasized the life history of single species and have not incorporated either interaction with other species or spatial distributions.

Most published models of complete animal communities have consisted of a set of simple differential equations which is used to represent energy transfers between grossly defined trophic levels. The following system of differential equations is given as typical of those employed to represent production of plants and animals per unit area of surface. Note the linear food chain assumed (phytoplankton → zooplankton → forage fish → carnivorous fish). The dot indicates a time derivative.

$$\dot{P} = P(c_1 I T g(N) - c_2 Z - c_3 - c_4 T)$$

$$\dot{Z} = Z(c_5 P - c_6 F_1 - c_7)$$

$$\dot{F}_1 = F_1(c_7 Z - c_8 F_2 - c_9)$$

$$\dot{F}_2 = F_2(c_{10} F_1 - c_{11})$$

$$\dot{N} = c_{12} f(t) - c_{13} P + c_{14} Z$$

where P is phytoplankton, Z zooplankton, F_1 forage fish, and F_2 carnivorous fish. (Common units for these entities are calories, grams of carbon, or grams of dry or wet organic tissue). Here N represents general nutrient abundance, e.g. average phosphate concentration assuming some fixed ratio between phosphorus and other elements; $g(N)$ is a positive, non-decreasing and asymptotic function of N while $f(t)$ is a function describing the changing rate of nutrient import with season or exogeneous factors. The c_i for $i = 1,\ldots,14$ represent numerical constants with appropriate dimensions. For example, c_2 is the grazing coefficient or instantaneous rate of removal of phytoplankton per unit of zooplankton. I and T are exogeneous variables representing incident radiation and temperature, respectively. These are usually cyclic functions of time.

The validity of models of this type rests upon the following assumptions:

(1) The trophic levels specified can be defined and measured; matter or energy flows only along the pathways indicated.

(2) All important organisms are included in the model.

(3) Growth and reproduction can be combined in general production coefficients and natural mortality and respiration in general loss-rate terms.

(4) One nutrient acts as a controlling factor or meaningful index in the ecosystem.

(5) The form of the functional relationship between productivity and the physical factors is approximately correct.

(6) The ecosystem being studied can be treated as an isolated and homogeneous unit.

Methods of solving these equations range from use of analog computers to various ad hoc procedures that arbitrarily assume existence of some sort of steady-state conditions. We are not aware of any studies that include a truly rigorous statistical comparison between results predicted by this type of model and field or laboratory observations. There have been many crude comparisons between values calculated from ecological models and observational or experimental data. However, because of serious deficiencies in sampling and data collection and simplifications introduced to render the system of equations more tractable, these comparisons cannot distinguish between different, remotely plausible hypotheses of ecosystem behavior.

Certainly, the past accomplishment of ecological models of this kind is to have provided insight into the organization and functioning of ecosystems; it is doubtful whether some of the present concepts could have been developed in the absence of these models. The models have served also as a fertile source of ideas for laboratory experiments and the design of field sampling programs. The models have further served the usual purpose of mathematical models in synthesizing fragmentary studies and providing a focus for diverse experimental work.

One of the most successful practioners of this type of modeling is Riley (1963, 1965), who examined steady-state solutions for models of biological productivity and applied these solutions to field observations taken under quasi-steady-state conditions in different regions of the ocean to solve for model parameters. Riley's model seems to provide useful estimates of steady-state concentrations of phytoplankton, zooplankton and phosphate. Steele's 1958, 1961 and 1965 papers, as well as that of Dugdale and Goering (1967) should be consulted for further variations and extensions of this general approach. Parker (1968) modeled the response behavior of biological productivity in Kootenay Lake to a reduction in the amount of inorganic phosphate pollution from a fertilizer plant located near the Kootenay River above the lake. Parker integrated numerically on a digital computer simultaneous differential equations representing rates of change in phosphate concentration, algae concentration, cladoceran density, and kokanee standing crop. Seasonal changes in river discharge and phosphate concentration, lake temperature and phosphate concentration, and photoperiod are included in his model. Parker does not claim a high degree of realism for the results he obtained.

A number of large-scale biological modeling projects have begun recently. Many of these projects may involve concurrent field and laboratory studies, but at the heart of each is a large computerized digital simulation model. The use of simulation is becoming so widespread that there can be little doubt that it will be a standard ecological research method in the future.

The largest ecological simulation modeling efforts in the United States are currently supported by the National Science Foundation as part of the U.S.'s participation in the Analysis of Ecosystems Integrated Research Program of the International Biological Program. Each of the main modeling studies is associated with a particular biome. Studies of the Grasslands biome and Deciduous Forest biome are now receiving major funding. Four others, Coniferous Forest, Desert, Tropical Forest and Tundra biome studies, are in various planning stages. N.S.F. also is funding a modeling study on the biological productivity of upwellings in the sea. No aquatic or estuarine biome studies are being supported on a scale comparable to the

Grasslands or Deciduous Forest biome studies. However, many of the current and proposed modeling efforts are directed at developing basic conceptual approaches to ecosystem modeling and modeling methodology. The N.S.F. programs are extremely broad and coordinate various types of field work including experimental manipulation of ecosystem components with laboratory studies and computer modeling and simulation. Research in each of the biome studies is classified into three main categories: major site studies, process studies and biome-wide studies.

Currently, there are several numerical modeling studies of lakes in the United St and in Canada. One of the most ambitious of these, the total systems study of Lake Wingra a multidisciplinary group at the University of Wisconsin (Watts and Loucks 1969), is being incorporated into the Deciduous Forest biome program as a major site study.

A particularly intriguing model-building exercise is that of the Environmental Systems Group of the Institute of Ecology at the University of California at Davis. This group is attempting to construct a simulation model of the human society and environment of the State of California (Environmental Systems Group 1969).

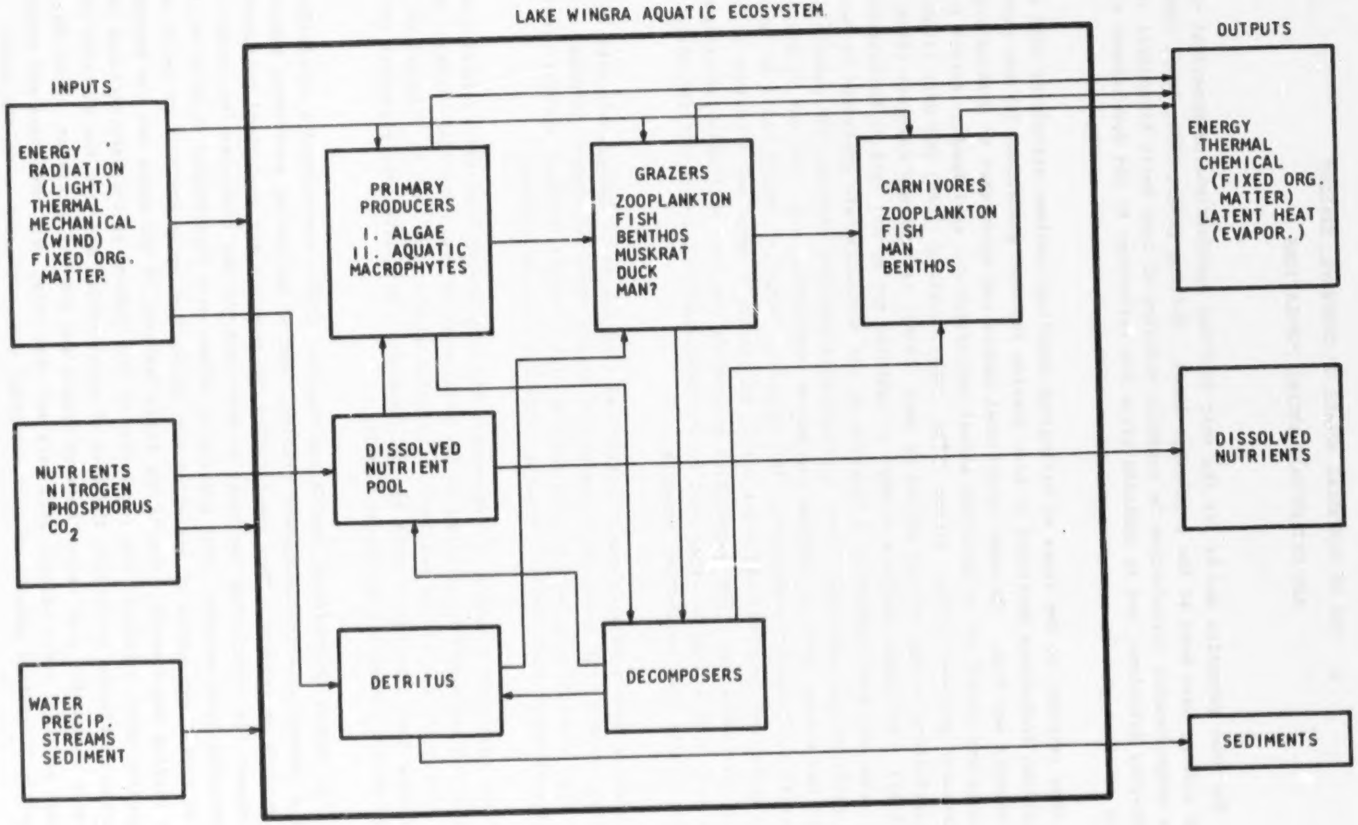
LAKE WINGRA AQUATIC ECOSYSTEM
INPUTS
ENERGY
RADIATION
(LIGHT)
THERMAL
MECHANICAL
(WIND)
FIXED ORG.
MATTER
NUTRIENTS
NITROGEN
PHOSPHORUS
CO_2
WATER
PRECIP.
STREAMS
SEDIMENT
PRIMARY
PRODUCERS
I. ALGAE
II. AQUATIC
MACROPHYTES
GRAZERS
ZOOPLANKTON
FISH
BENTHOS
MUSKRAT
DUCK
MAN?
CARNIVORES
ZOOPLANKTON
FISH
MAN
BENTHOS
DISSOLVED
NUTRIENT
POOL
DETRITUS
DECOMPOSERS
OUTPUTS
ENERGY
THERMAL
CHEMICAL
(FIXED ORG.
MATTER)
LATENT HEAT
(EVAPOR.)
DISSOLVED
NUTRIENTS
SEDIMENTS

Fig. 8.1 A compartment model showing (1) the major inputs, (2) the pools of plants, animals, dissolved nutrients and detritus, and (3) the major outputs of an aquatic ecosystem. After Watts and Loucks (1969).

3. USE OF NUMERICAL MODELS TO CONSERVE, EXPLOIT AND EXTERMINATE ANIMAL POPULATIONS

The most extensive and by far the most fruitful applications of numerical modeling in applied ecology have been at the population level. Holling (1963, 1964, 1966, 1968, 1969) provides a comprehensive introduction to computer modeling of such basic biological processes as predator-prey relations, and in addition gives key references to the development and the application of strategies to control populations of insects harmful to man.

More relevant to the types of biological modeling problems associated with estuaries are the modeling techniques developed to help provide rational guidelines for the harvesting of marine mammals and fish. The more traditional models and approaches to determining the "maximum sustained yield" of an exploited animal population are explained in detail in the books by Beverton and Holt (1956), Ricker (1958, 1966), Gulland (1969) and Watt (1968) and by many contributors to the volumes edited by Watt (1966), Le Cren and Holdgate (1966) and Van Dyne (1969). The usual analyses attempt to maximize the annual rate of harvestable biomass or value-adjusted biomass as a function of the mortality rate generated by harvesting and of the earliest age exploited. More sophisticated analyses consider the possibility of differential harvesting rates on various population components, e.g., the use of age-specific or sex-specific exploitation techniques. The harvest of Pribilof Island seals is taken primarily from three- and four-year-old males unable to acquire a harem and therefore no longer essential to the population. The unqualified success of the internationally supervised management of the seal herd is due in large part to the development of a mathematical model which realistically mimics seal population dynamics.

Existing models usually employ historical time-series of demographic data on population fecundity, growth, and mortality to establish steady-state management programs. These models have been successful primarily when dealing with a single dominant species under environmental circumstances that dampen excessive variability in recruitment.

There have been a number of large-scale and complicated simulation models constructed to solve biological or economic problems in the management of exploited fish stocks. Up to the present, virtually all of the realistic simulation models have been so directed at solving specific problems that they have little general interest. Extensive bibliographies are given by Newell and Newton (1968) and by Paulik (1970).

Royce, Bevan, Crutchfield, Paulik and Fletcher (1963) constructed a simulation model to represent a common estuarine management problem, that of harvesting anadromous species as they travel through an estuary. They investigated the economic and biological consequences of various schemes for restricting the entry of gear into the net fisheries for salmon in northern Washington State waters. Four species of salmon were represented in this model and their rates of travel and routes of migration were determined by an analysis of catch data as well as from tagging experiments. One of the basic features of the model was the management decision algorithm which simulated the regulation of the fishery by the International Pacific Salmon Fisheries Commission to control the rate of exploitation and also the division of the catch of sockeye salmon and pink salmon between Canada and the United States. Cost functions for three types of gear, purse seines, gill nets and reef nets, were developed and potential economic benefits of various amounts of gear reduction were estimated using the model.

4. RECOMMENDATIONS FOR BIOLOGICAL MODELING IN ESTUARIES

In the immediate future the most useful numerical models of biological phenomena in estuaries undoubtedly will be concerned with certain "key" species whose basic life characteristics are fairly well known. While it is clear that models capable of representing the dynamics of entire communities of animals in estuaries will evolve in time, major research efforts comparable to the National Science Foundation's biome studies will be essential for their development. It is almost impossible to estimate the length of time required for the development of realistic and predictive general estuarine ecosystem models. Certainly, much depends upon the possibility of "breakthroughs," especially in the area of methodology in the Analysis of Ecosystem Integrated Research Program. The feasibility of a major Estuarine biome modeling program should be investigated.

4.1 KEY SPECIES MODELS

Although the immediate feasibility of total ecosystem models is questionable, extremely useful simulation models of certain important estuarine animals could be developed using existing data and techniques. Considering their potential usefulness, the lack of interest in such models is surprising. The following steps are necessary to develop a simulation model of important estuarine species:

(1) The general characteristics of life histories have to be determined and the major predator and prey species at different life histories established.

(2) Basic biological processes in the life cycles have to be modeled. Data from isolated individual experiments should be synthesized by means of mathematical models. The types of processes of special importance to estuary-dependent species include:

(i) synergistic physiological responses as a function of simultaneous exposure to multiple stresses at different levels of critical parameters such as temperature, dissolved oxygen, turbidity and salinity;

(ii) spawning requirements, and tolerance ranges and optimums for chemical and physical variables;

(iii) larval behavioral responses to flow conditions and to such factors as dissolved oxygen and total dissolved solids;

(iv) migratory behavior and effect of environmental gradients on movements;

(v) growth response as a function of quantity and quality of nutrient supply under different environmental conditions; and

(vi) normal mortality rates and mortality response to environmental pollution.

Many of these processes would be expected to vary with intrinsic characteristics of the animal. Thus, the model should include population structural characteristics such as age composition, sex ratio, and spatial and temporal segregations of identifiable groups.

(3) Submodels of fundamental biological processes are combined in life history structures and with sectors containing hydrodynamic submodels to determine values for physical and chemical parameters. The biological sector of the model would be used to forecast responses of populations of key estuarine species to alternative management policies.

One of the most important uses of an estuarine simulation model is simply basic bookkeeping on duration and intensity of exposure to various stresses for transient populations and in a highly dynamic environment. Even if behavioral information is not complete, exposure boundaries can be established. Calculations involving multistage reactions, e.g. sequential decision-making as occurs in directed migrations in which movement is affected by local conditions, are practical only when using a computer simulation model.

Modeling can effectively complement biological surveys and long term baseline studies in unpolluted estuaries. The interaction between modeling and biological observation should accelerate the model development.

Modeling of key species should include the effects of events occurring outside the estuary on the abundance of transient animals. For certain important species, extensions of the model to include economic factors such as the values of different spawning areas in an estuary should be straightforward. In the area of forensic ecology, legal arguments involving water quality standards are far easier to arbitrate directly in terms of economically important animals than in terms of surrogate measures. Of course, the first objective of such a modeling effort should be to summarize life history data in a form that makes them easily manipulatable and accessible to estuarine managers.

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CHAPTER IX

DISCUSSIONS

1. ESTUARINE HYDRODYNAMIC AND WATER QUALITY MODELS

THOMANN: I want to support very substantially Dr. Harleman's suggestion that we should get on with looking at some of the sources and sinks. From my own point of view, I would say the state-of-the-art of water quality modeling is to the point where the hydrodynamics of the system generally--now there are exceptions--are of less importance to us, in the sense of our ability to understand what's happening, than the sources and sinks and the interaction between some of our variables.

I think we know very little about some of the interactions that are going on, the order of the reaction rates, the linear versus nonlinear reaction systems. The distinction between sources and sinks, and reactions here, I think, is well worth making. Feedback effects, for example, we know very little about. Now they may be imbedded in some hydrodynamic system, but I think the state-of-the-art of describing the hydrodynamics of the system is so much ahead of our ability to describe these interactions that we need much more work in those areas. I think that when we get to the order of some of these reaction rates, even in a first-order system, that we find, by and large in many applications in water quality analysis, that the system is very responsive to the order of the reaction rate and much less so to the details of the hydrodynamic system itself. Reaction rates occur, for example, that are orders of magnitude greater than generally what was used in Dr. Harleman's review here, and that may alter the way one looks at some of these profiles.

So I would certainly agree that we need to move on with some of these studies, to take a look at sources and sinks, and interactions.

O'CONNOR: Are these hydrodynamic models really necessary to answer some of the quality problems that we have?

CALLAWAY: In modeling the Columbia, what we're trying to do is solve this equation:

$$\frac{\partial T}{\partial t} = -u\frac{\partial T}{\partial x} + \frac{\partial}{\partial x}\left(E_x\frac{\partial T}{\partial x}\right) + \Sigma S$$

You will notice that this velocity term is an input to the temperature model. We've gone to a lot of trouble just to get the intertidal velocities.

O'CONNOR: Yes, that's what I mean. We've gone to a lot of trouble just to get one number. Is one number that critical to the problem you have here?

CALLAWAY: Yes, I think so.

O'CONNOR: We can use an equation like this to clarify a point. That E includes a lot of garbage, a lot of things. You take the equations that you've worked with, and you lump all of these effects together into the diffusion.

RATTRAY: The point being that those different things you lump together are lumped together very differently for different river flows, or winds, and so on.

O'CONNOR: That's correct, and you can get an empirical correction of that E with the Q plus the width, and so forth.

Seeing the relative importance of these things is one of the more important things we have to do in an estuary, the relative importance of the hydrodynamics versus the kinetics of the reactions, and I, right now, am undecided as to how to pursue research on this point. This is one of the big questions we face. I realize that these both are going to go ahead simultaneously, but I would like to get some feeling for the relative weight of the kinetics versus the hydrodynamics.

HARLEMAN: I think the point really boils down to the fact that in most of these water quality models there are variable coefficients or knobs that one can turn, most of them related to reaction rates. It's always possible with any model, even the most crude one, if you have enough knobs to turn, that you can match a set of data. I think it's very important to remove as many of the knobs as we can, so that the final ones which are left to turn are really related to the ones that we have no other way of finding by analysis. Really the whole point of this discussion, as I see it, in my portion of Chapter II, is related to removing one of the knobs, and that is dispersion. I think we should get on and twist the knobs relating to everything else, but not twist that one, because when you twist that one you change all the others. And if you are ever going to find anything fundamental about such basic things as even the rearation rate in an estuary, we've got to have less knobs to turn. Otherwise, we're just finding an adjustment of a multitude of parameters which fits a set of data. If you change anything in the system then to try to predict, all you can do is keep all the knobs the same.

THOMANN: But it turns out when you turn some of those knobs the system behaves quite differently than when you turn other knobs.

HARLEMAN: Well, I'm just saying we should reduce the number of knobs. Let's reduce the hydrodynamic knob.

THOMANN: No disagreement with that.

HARLEMAN: In your discussion of the tidal advective models where you get down to talking about whether they should have four or fifteen time steps per day, it seems that you have to be precise of what it is you are talking about in the advective term. You can't just write down the conservation of mass equation with a dispersion coefficient and by any means assume that that dispersion coefficient is a parameter which you can pull up, because it depends on how you define all the other terms, and, as I have already said, the importance of it changes as you change the definition of time scales.

JAWORSKI: On the Potomac we've got the advantage of applying both the Orlob or "real time" model and the Thomann or "tidal average" model. One thing about the tidal-average approach is that one can perform sensitivity computations very cheaply. In some of our work we can tell if we have to go to a real-time solution just by varying the dispersion and testing the sensitivity. This is very simple. So I think using the tidal-averaged model for the DO-BOD reaction system, which has high rates, is at times a very uncomplicated method of getting a fast answer and order of magnitude.

The opposite appears to hold for nutrient transport systems. We are working trying to model nutrient transport on an annual flow cycle. We are running into trouble using the tidal-averaged model over a range of flows while keeping constant the dispersion coefficient. I think the applicability of either the tidal-averaged or the real-time model comes in in what kind of answer you want and what you're willing to pay for it.

HORNE: In this quick sensitivity test, you are saying to turn the dispersion knob?

JAWORSKI: Yes. We'll run various tests with the Thomann model just to see how sensitive it is to dispersion. On the work we just finished doing, we found for low flow range the predicted profile was the most sensitive to the decay rate. The same thing was observed using the Orlob approach. So there it didn't matter what you were using, a tidal-average or a real-time model, you've got to know the reaction rates.

THOMANN: To reinforce that, in some of the algal modeling we've been doing, plankton modeling, we have growth and death rates of 2 per day, so we're up another order of magnitude from the .2 or .3. The system tends to be almost completely dominated by what's going on in those kinds of terms.

JAWORSKI: At high decay rates, we've varied the longitudinal dispersion in the average tidal models from 1.0 to 6.0 sq. miles/day and obtained similar profiles, depending on the hydrologic conditions. We get approximately the same answer in the real-time model. I think in the BOD-DO sag relationship it's more important to define the reaction rate than the hydrodynamics.

WASTLER: Yes, but, depending on your model (and I don't want to get into the merits of various models), if you don't know what the relationships are about the BOD decay rate and the hydrodynamics, if you are just going to the curve-fitting and the knob-twisting routine, what you don't know about your dispersion coefficient will appear in your BOD decay rate.

THOMANN: Not in the same way. Absolutely not.

WASTLER: Yes, but in an entirely unpredictable way.

THOMANN: You can't arbitrarily turn those knobs and expect to get exactly the same responses. As I pointed out, the decay rate acts as a multiplier in these systems, not in the same way as dispersion. I think the point is that the equations show there isn't an equal trade-off in the solution of the equations with E as there is in K. I think they behave quite differently with responses to changes in K as to changes in E. One interesting way to look at that is to start from the conservative salt balance equation where K is 0, and just put in a little bit and you get a fair amount of reaction response. Generally, the responses are quite nonlinear with respect to that reaction coefficient. Quite nonlinear.

HARLEMAN: I think if you get into salinity regions it's always going to depend on dispersion quite heavily. I don't think that on a one-dimensional basis you can really ever discount that. Only if you're in certain regions, I would agree with you. But, in general, you cannot discount that.

THOMANN: No, I'm not discounting it. I'm saying that the solution response is relatively insensitive to it, over a wide range of our choice of that coefficient. No, it definitely has to be there, but I'm saying that a solution response in highly reactive systems is relatively insensitive to that coefficient, and it may be worthwhile to trade-off that time-dependent model for that coefficient.

HARLEMAN: I said in the conclusions of my chapter that there was a place in the future for both of these models. Really, I think all we really need to be concerned with is that we know what we are doing, and I can see a very good place for calibration of the non-tidal advective model using the real time model. In other words, you do a brief study using the real time models to determine some of the grosser effects of nontidal models. You do a numerical study instead of a field study, which ought to be a gain in time and cost. So there is a place for both.

BAUMGARTNER: Dr. Pritchard brought up the problem of disregarding the vertical eddy diffusivity on the basis of what looked to be a uniform distribution vertically of salinity, and there was some agreement that this was important. And what I want to do is ask, if possible, to show some comparison of what kind of difference this might make in the Mersey or the James River, if you have any examples, where the concentration would be an order of magnitude, or 10%, or how much different if that assumption was embraced and if it was not.

PRITCHARD: Well, I can give you some examples which draw on biology rather than chemistry of the environment. I don't think a model has been run for the Mersey or the James in which one neglected the shear terms, or did not neglect them. But if you take, for example, small organisms that are essentially carried by the water and consider this as a pollutant or an indicator, that is, some component which naturally stays in one place or moves and its movements are controlled to a good extent by the same processes that control the distribution of properties, and realize that if you did not have the shear term, the distribution that you observed couldn't possibly exist. An example of this is, and here I'll go to a larger body, the Chesapeake Bay, which is in many ways just an enlarged James as far as the terms that are important in it go, the hard-headed croaker, which is a major winter food for striped bass. The croaker spawns off-shore, in the fall, just about the time when we begin to get overturn in the temperature structure, and it seeks the warmer water, which is now not at the surface but near the bottom, and as a consequence is brought up the bay. These are little fingerlings, so long. They can't direct their migration up the bay. But in two months after they are born, we find them in the deep holes right up where the striped bass are wintering, and they're food. Now again it so happens if you compute transport time of a particle which stays in that part of the structure that has an upsteam motion it gets there in two months. So these organisms are using this flow pattern to its fullest in moving into a nursery area, besides their being food. In a one-dimensional model you couldn't predict this.

BAUMGARTNER: I think that's an example of what Dr. Harleman said, that if it isn't one-dimensional, don't try to use a one-dimensional model.

PRITCHARD: We might look at perhaps some experiments with tracer materials, remembering that in Don's examples here essentially the upsteam extension from the source is about a tidal excursion in some of the cases, where we'll find the upstream excursion of a pollutant to be many tidal excursions. Now I don't know how much of this will affect the local concentration near the point of highest concentration, but it certainly affects a lot of trends.

HARLEMAN: Those examples were in the nonsaline portion, and if you get into the larger dispersive zones then you will find it more than one tidal excursion.

BAUMGARTNER: This is the kind of comparison I'm looking for, if we can provide something for the record to show what the magnitude of our concern is, if we happen to be trying to model concentration of some pollutant or some water quality parameter, whether it is an order of magnitude or ten percent or whatever it is.

PRITCHARD: Let me say this then. I think that certainly the effects of the vertical shear can be modeled by some sort of dispersion coefficient. The shape won't be exactly the same as occurs, but it grossly can be modeled by some sort of dispersion coefficient. And the question I would make is, just as in the case of the two-dimensional systems or one-dimensional systems which are sufficiently uniform over a cross section or in the vertical, where you find if you look at more detail in the time-dependent horizontal velocity field you don't have to worry about the dispersion coefficient, if in the same way you look at more details in the vertical structure, maybe you don't have to worry so much about some of these diffusion terms.

RATTRAY: For a number of classes of estuaries, the longitudinal salinity distribution is basically governed by the one-dimensional model, although in the local salinity change the horizontal diffusion term is really a small part of the local salt balance. This means that whereas you can do a reasonably good job of cross-sectional mean salinity determinations with the one-dimensional model, other kinds of distributions that are not put in in the same way, essentially over a cross section at the seaward end, but more local sources, are not going to be nearly as well described in the one-dimensional model. This is a real problem if you're talking about something other than salinity, or other than simple sources.

WASTLER: Would it be possible to get some criteria about under what conditions you would use the one-dimensional versus the two-dimensional versus the three-dimensional, or at least some guidelines as to how such criteria should be set up?

HARLEMAN: I think it's a question of availability at the moment. It isn't really one of just making a choice.

PRITCHARD: Right.

WASTLER: Well, certainly there is some criterion which makes you recognize that it's a two-dimensional problem versus a one-dimensional problem.

HARLEMAN: If you have an embayment then obviously this is not one-dimensional, no matter how you cut it. Just by looking at the geometry you can see that the major directions of flow are simply not going to be defined by one dimension.

WASTLER: Certainly, but what we need is an explicit statement of that. This is a very real and very critical problem, at least from my standpoint. When we are being asked to evaluate certain types of models in certain types of estuarine systems, it would be very nice to have some kinds of guidelines to make a judgment as to whether there was a reasonable chance of a particular model actually being useful. It should be possible to at least lay it out to such an extent that the additional information could be gathered to make it quantitative.

RATTRAY: Well, you're asking really a very multipronged sort of question. In terms of salt flux, I can give you a pretty good answer, but in terms of something that has a half life of a few days, that's a much more complicated kind of a problem. For the kind of a biological organism that has the behavior that has just been described, you'd have one set of answers, and another set if you're talking about something with a different time frame and spatial frame and scale distribution. An estuary you might have treated one-dimensionally would have to be treated two-dimensionally, just because you are looking at, in the same estuary, a different phenomenon. It is fairly complicated.

THOMANN: There are some situations where, even though there is an embayment involved, the extent of tidal mixing is so great that for a particular water quality variable one is studying it may be useful to consider the entire bay completely mixed, and look at the dynamics of what is happening as far as growth-death. That is, physically it may have all the features of a two-dimensional system, but for the particular problem you are looking at, you might just get away with a simpler representation.

PRITCHARD: You don't really care about the horizontal-vertical variation in the water quality structure. You care about what that does to the system. So you treat this as a mixed bucket with inputs and outputs and what happens in the middle.

THOMANN: That's right, and what happens in the middle is where you bring to bear all the knowledge you have on the dynamics of fluctuations, prey-predator relationships, and all that.

PRITCHARD: And they are probably much more important than the differences you get out of the hydraulic system.

THOMANN: Right.

LEENDERTSE: Actually, in a three-dimensional model, you need to know what are the largest contributions of terms that go into it, then you can make your selection. So if you have very rapid decay rates, you need to develop them more. Hydrodynamically, in the horizontal you can make a distinction in two ways, I would say. As soon as the flows are not predominantly unidirectional, but the terms start turning around, then you can say you need definitely a two-dimensional model. Also, you very likely need a two-dimensional model when you have tidal flats. But to give you a meaningful list, we'd have to go, at least I'd have to go, to a certain number of estuaries and see what their main characteristics are.

WASTLER: What you just said is perfectly satisfactory from the standpoint of what I was trying to get at.

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PRITCHARD: I would like to make one other comment with respect to things that ought to be done, and that is, again depending on where you are, your awareness of the concerns and certain aspects of the problem vary. I've been working in a very large estuary, where, if we look at its total assimilative capacity, the total capacity is quite large. I don't find the problems for which any of these models would really be very pertinent. I can on a very simple basis determine how much diluting water is available and we could make use of. And the real pollution problems that we face are generally local in character, that is, peripheral tributaries, small embayments, that are badly polluted because they don't flush with the less-contaminated water in the larger bay. Where discharges go into the larger bay, the problems have been to develop ways to make use of the diluting water. So we face engineering design problems of how to most effectively use the capacity of the system, both the diluting capacity and in some cases the capacity of the system from standpoint of non-conservative losses of some of the material.

This is very true, say, in the case of some of the thermal inputs. The problem with a big power plant like a nuclear plant is not this large-scale problem in which one can show how the pollution distributes up and down the estuary in a one-dimensional sense or even in a two-dimensional sense (where we are now looking at two dimensions vertically, not horizontally). This is a relatively minor problem. The heat is spread a hell of a distance, but at very, very low temperatures like a few hundredths of a degree, up and down the estuary. The problem is that in the tidal segment adjacent to the plant site you've got potentially a pretty steady supply of about 90,000 cubic feet a second. If you could make use of that, if you could design the input to take advantage of this, you can get temperatures down to 4/10ths of a degree or 6/10ths of a degree due to dilution very fast. For many of the problems that we've faced, our problems of design of intake and discharge structures make use of the diluting water.

From the standpoint of site location for such systems, the desire is to find sites which have potentially large diluting capacity. This means that narrow streams or the upper reaches of estuaries aren't very good sites, but for large estuaries, well down in the estuary may be a good site. An open coastline may be a good site if you make use of the diluting water by proper design. In many cases the work of Don and other people on dispersion for horizontal jets becomes very important. The effect of longshore currents upon the entrainment of momentum jets is a very important term which potentially has large diluting capacity, if you could make use of that. Also large tributaries from which you can dissipate the heat from regions of very low temperature excess. In the thermal modeling that I've been doing, I have found that these are the pertinent things and not the gross or large-scale distributions.

THOMANN: Yes, but the point there is that the physics of heat are quite well understood. I think here, while there may be a design problem associated with dilution effects to disperse the effects of heat, it's that link between heat and what happens in the higher-order ecological system that really is where we're hung up badly.

PRITCHARD: Yes, but the link is through temperature, not through heat. What I'm getting at is that you want to dilute the heat.

THOMANN: But we don't know that. I think that's the problem. We don't know that hundredths of a degree may not make a difference.

PAULIK: It seems that one of the problems is that matter of basic objectives.

PRITCHARD: But it's still in terms of degrees, not BTU's.

HARDER: That hundredth of a degree might be the difference between a cloudy and a sunny day. I'd like to suggest that in terms of the natural variations that this hundredth of a degree may not be important.

THOMANN: In terms of this temperature excess problem, we ran a whole time series analysis on temperature. Background variance that is generally unexplainable runs on the order of at least a degree. All tests indicate somewhere on the order of a degree.

EDINGER: I'm surprised it's that low.

PRITCHARD: Yes, I am too.

THOMANN: That's absolutely the last little bit of variability that is completely unexplainable.

EDINGER: You mean in terms of periodicities?

THOMANN: Yes. In terms of any periodicities. Just background noise.

PRITCHARD: We did a field study of the Chalk Point plant for something like a nine-day period. Within that nine-day period, our best estimate of the background temperature showed diurnal and tidal fluctuations for a total range of 9°. And we're looking at 12° temperature.

HARLEMAN: And you're limited to 1½°?

THOMANN: That's why I brought up the mention of degrees. I understand some of the requirements are on the order of one degree, and background variability, strictly background noise, is on the order of a degree.

PAULIK: I'm disappointed we haven't mentioned any of the biological criteria, because I think that's the thing that generated all the current interest in temperature. If, as Dr. Edinger mentioned, salinity is the most important factor determining the density structure of an estuary, certainly the temperature is a critical thing in determining its total biological characteristics. And the local temperature distribution is just exceedingly important. Even though we get a lot of variability, especially on the east coast, I think some of the west coast estuaries are very stable in terms of temperature structure. Many of the organisms, especially the economically important organisms like oysters and salmon, are keyed to the specific temperature, and their whole life cycle depends on this temperature being realized within a certain season. Temperature controls the spawning of oysters. Just a few degrees will trigger the oyster spawning. It certainly controls the return of salmon to certain streams. I feel that this should be given some emphasis in the report, especially the local effects of temperature below some discharge point, because the importance of the local spatial distribution of temperature cannot be overemphasized.

EDINGER: You know, when we began in this heat business--sometimes I wonder why--about eight years ago, we were pretty naive looking back now, but one thing was obvious at the time, and that was the fact that we might be able to come up with the best temperature prediction methods in the world if we put enough money into it, but the one big job was to have some method of getting this interpreted. Can the biologist give us some idea of how much detail he needs in terms of a temperature distribution so that he can make that interpretation? Then we can go ahead and make our predictions fit them. This, to me, would have been the criterion. And after eight years of working on a number of studies in which very competent biologists have been involved, I don't think we've met this criterion yet. I'm not about, myself, to undertake a discussion of the effects of temperature on organisms.

PRITCHARD: Here again, it depends on where you are. It seems to me that this is not part of the modeling. It's what you need to know in order to say what the effects of any discharge are, and in order to get the criteria on what this discharge means. I don't think it's part of the state-of-the art of modeling.

PAULIK: Well, I think this is where our modeling should be going.

PRITCHARD: Well, I agree, and I think the state-of-the-art is pretty damn poor.

PAULIK: It's pretty poor, but I don't think we're using the information that we have available.

EDINGER: Let me ask the question this way. I heard this morning some estimate that someone wanted to know temperatures within .01 degrees, I hope centigrade. This is to do with the data question we were discussing. My feeling is that we can hit temperatures within a couple of degrees depending on what you want for spatial detail and depending on what you want for temporal detail. On temporal detail it becomes a function of your input data. How good is your meteorological data, and how much experience have you had working with this particular set of data? Now you take a guy and sit him down and let him run through a set of data, once even making a forecast, then let him go back and make a hindcast. His second time through on his forecast he'll be pretty darn close to those records. How good is your boundary condition data? You see, the question here is what do you feel you need for detail in terms of temperature distribution? I think you're going to have to admit that you're going to have to answer this almost case by case, knowing the existing waterbody, knowing habitat areas, and things like this.

PAULIK: I think you have to look at the particular organism that's going to respond. You might do things like make on-site tests of the water under different temperature conditions, and possibly set up some sort of a physiological lab at the site. But then your model should be able to incorporate that information and use it to forecast.

PRITCHARD: Well, it seems to me that you don't have to incorporate a biological model into the temperature model. You predict the distribution of temperature, and then you take that and predict the consequence of that with a biological model. Now, to give you an example of a very simple way of approaching this, if we look at, say, the Chesapeake Bay, one can look at Maryland and say that there are certain plants that raise the sectional mean temperature or the temperature in the tidal segment opposite the plant site by four-tenths of a degree. Now you want to know what that means. It displaces the time curve by that amount, really. And one way to say what it means is to say, where do I have temperatures like that? I've just got to move to the south end of the bay, the Virginia segment of the bay, where the mean annual temperature is eight-tenths of a degree higher than the Maryland section of the bay. And I've got a model.

PAULIK: It's nice to have control. Right.

PRITCHARD: But the thing that we've imposed on those relatively small differences is the fact that the annual temperature varies at one place during any month of the year, from one year to another, by a range of six-and-a-half degrees.

PAULIK: Well, that's in this particular area. Maybe you have eggs, say, of some particular organism that are going to be down there for two months. So they integrate the temperature essentially, and have a so many day-degree requirement to hatch. That will integrate out a great deal of the variability that you're talking about. You might have some sort of biological stabilizing thing.

PRITCHARD: Well, a warm year would be warmer somewhat, and a cold year would be colder somewhat. I've seen fourteen years out of a fifty year record where the average temperature was a degree-and-a-half higher than the fifty year mean.

PAULIK: Well, maybe in that case you need the variability of temperature itself.

PRITCHARD: No, you don't. You don't change the time fluctuation whatsoever. You just change the mean. But I think there are models that you could look at in nature.

PAULIK: Well, maybe we should set up some as control.

PRITCHARD: These kinds of studies have been going on. And at the end, you say "What did you find out?" They say, "We found the environment is variable." And that the organisms vary and the response varies, and that's about what they found out. It's been a very disappointing experience over the years.

PAULIK: I'll agree with that, but I think we are beginning to accumulate the type of physiological background that we need to begin to incorporate some of these factors into the model. I see no reason why the model shouldn't include, or at least plan to include, biological responses.

EDINGER: There is no reason why it can't. Because here's your temperature prediction and it's not going to be influenced by the organisms unless you put a whale in there or something. In other words, the temperature is independent in a sense that I don't think we have to worry too much about it influencing the dynamics, except locally near a discharge where it will stratify.

PAULIK: But, how do you know how much detail you'd like to put in until you try to put some of this into a biological model and see what the response is, to help you determine your criteria? This is what you need. Otherwise, it's going to be determined on a political basis.

PRITCHARD: It doesn't have to be this particular model. It needs to be a model that takes the temperature distribution and predicts what it means to the biota.

The important thing in temperature is the time response. We can show for instance that some of the organisms drawn through the condensers at Chalk Point are killed. There is a certain fractional mortality of passing through that plant, which discharges to a 7,000 foot canal and takes two-and-a-half hours to discharge with virtually no temperature loss. So they're raised 11.4 degrees above ambient for two-and-a-half hours. Now that's quite different than if they're raised 10 degrees above for four minutes. Then the discharge undergoes very rapid dilution and temperature decrease. Where oyster larva are killed going through the Chalk Point plant, in a plant that is designed to minimize the time of contact, the oyster isn't killed.

PAULIK: Yes. I agree wholeheartedly.

PRITCHARD: These kinds of experiments are being run for that kind of simple model. It's a fairly simple question you're asking. You're not asking what happens to the migration of shore fish past a plant. That's a very much more difficult one.

PAULIK: You can, say, put an envelope of the minimum-maximum exposure, and put a time factor in for a migratory fish. If he has to migrate by this plant within a certain period of time, he takes the route that will minimize his temperature increase exposure, or he takes the route that will maximize it. At least you can involve things like that, which are really difficult to compute without models or without incorporating hydrodynamic factors or temperature.

PRITCHARD: Well, we haven't had the expertise on modeling in the biological field that we need.

ESPEY: Do you think the sources and sinks in the temperature model such as longwave and shortwave radiation are fairly well-defined for estuaries? These empirical formulas that have been studied on freshwater reservoirs, how about their application to estuaries?

EDINGER: I haven't gone into that problem explicitly, so I really can't tell you, except we would be hiding ignorance on evaporation in the same empiricism in an estuary that we do on fresh water. I don't know, offhand, of any reason to believe that our rates should be any different, except for the fact that we probably get longer wind fetches and higher winds on a more open waterbody.

PRITCHARD: Given a wind and an ambient temperature, including the second order effects, humidity, etc you can predict the equilibrium temperature about as well there as anywhere and you can predict the driving function there about as well as anywhere, and certainly the surface cooling coefficient. I think now the uncertainties don't exist in that term, because the distribution within the area that are concerned is so dominated by dilution. If you're going to have a power plant that fits, that is, if it's designed so that it can go there, you've got to dilute. You can't depend on cooling. So you find that you could vary the cooling coefficient by fourfold and not get very significant differences in the distribution of temperature. In most real cases we find that 80% of the heat is lost at temperature excesses of less than one degree. So it doesn't matter much what size cooling coefficient you take in the part of the plume that you are concerned with.

I'm agreeing with what John has said, that we're now not concerned with hundreds-of-fold dilutions. We're being concerned with dilutions of the order of ten-fold. In that range, the temperature distribution is dominated by mixing, not by cooling. You get reasonable answers by neglecting cooling completely. And this is something that other people are coming very rapidly to the same conclusion. For instance, Parker's report of studies that have been done down at Vanderbilt, tells about systems in rivers where they got their prediction almost as good as what they observed in the river by neglecting cooling completely. Now, cooling has got to be the end product. It's sort of like molecular diffusion. It's got to be in there, but it's in there at some place where it doesn't matter as far as the predicting technique goes.

ESPEY: Well, in some of these shallow estuaries on the Gulf Coast, would cooling possibly be more of a constraint?

PRITCHARD: My point is that when cooling becomes a constraint, the plant is too damned big for that waterway. All you have to do is to compute the size required for an effective cooling pond, and you'll find that the areas contained within high excess temperatures are too large.

EDINGER: Well, though, there is another point in here. The way to double your rate of cooling is to double your temperature excess. And cooling pond design depends upon what temperature excess you want to operate your pond at above equilibrium. One way to get to small areas, if you're working in an area where you have, say, a mean weekly equilibrium temperature of 85 or 90°, is to operate your pond at 20° above that, with a 15° condenser rise, so that what's coming back into the condenser is 5° above equilibrium. In this case, you've doubled your temperature excess over that, which means you've confined your heat to a very small area, and you're recirculating it. The question is: do you want to take a shallow estuary and design it to be a cooling pond? If you're going to use it for that, design it to be that; the plant will be much happier.

PRITCHARD: Yes, but the organisms won't. I think one of the biggest misconceptions in power plant design that exists today is the concept that you gain by having regions of high temperature in a natural environment because those are the regions that you lose heat fastest. Because those regions are just going to turn out, with thousand megawatt plants, to be too large for the regulatory authorities to accept. I can give you case after case of the situation where you're talking about having temperature excesses, say, above 10° or above 5°, of thousands of acres, as compared to, if you design the plant right, of fifteen acres. And that fifteen acres is because of dilution, not cooling.

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PRITCHARD: I'm reminded of a study where we were concerned with a distribution around the discharge, and we were concerned with predicting the distribution within one or two tidal excursions, what the shape of the distribution was as it flipped around during the changing tide. But this concern was limited to something like one or two tidal excursions in a system that was maybe sixteen or twenty tidal excursions long. We weren't concerned with tidal times when we were looking at scales of 0 - 180 miles, only a sort of central mean. But we were concerned with tidal times when we were looking within plus or minus twelve miles or so of the system.

WASTLER: I think part of it goes back to the same scaling problem that Dr. Harleman pointed out this morning, with regard to the mathematical models. If you're using a broad-scale model, where you are talking about annual changes, you can't use it to look at the small scale variations, at least not with the same prototype data base. And the same thing with hydraulic models. If you build a hydraulic model at such-and-such a physical scale that you can look at the broad scale phenomena, the scale simply isn't right to look at the outfall locations. But you could do that with the physical model if you built a model, say, on the 100 scale.

HARLEMAN: The trouble is you have to build the whole estuary usually.

WASTLER: Right. So it lacks the flexibility that the mathematical modeling technique has.

RATTRAY: Well, you could do something. Some even fairly small-scale distributions may not be affected by horizontal turbulence processes. In that case, if you scale the vertical ones correctly, you don't really care that the horizontal ones aren't scaled correctly. They aren't important.

PRITCHARD: Yes, that's the point I was trying to make.

PAULIK: I think biologists kind of like physical models, especially if you model the local phenomena. You can apply your experience and observations to the model and get some ideas of how an animal might respond to a particular set of conditions. I worked on the Columbia River and several of the dam problems, and looking at the models there and the locations of the fish ladders has always resulted, I would say, in much better design. In fact, a couple of times we've gone to a model, after the ladder did not rate properly and were able to diagnose the problems. Occasionally the problems had been such that when the original design, for example, had spill gates located right next to a ladder and yet the ladder did not rate properly, going back to the model you could see what was happening and by changing the spill pattern you could get the fish to respond and use the ladder very nicely. The physical model seems to work with certain types of, say, local problems which mathematical models perhaps can't handle. It's one way of simulating what's happened in the prototype.

WASTLER: I think major structural changes, too, are something that mathematical models at the present state-of-the-art can't handle as well as physical models. Again, it's right back to the empiricism. You have to go on faith for every bit of it.

RATTRAY: Well, there's a difference between getting a qualitative answer and a quantitative answer, too. You can get a very good qualitative answer even if it's distorted.

PRITCHARD: There's a lot of difference in being able to take the city fathers out and stand beside the model and say, "Look, you put your outfall there, see the way the dye is going." There is that kind of demonstration advantage, which probably isn't worth the cost unless there is one of the models in existence.

LEENDERTSE: Don, I do not completely agree with you. You can do exactly the same thing with the mathematical model. I have made movies of mathematical models, and they are very instructive.

PRITCHARD: I would understand them. I'm not sure the mayor would.

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PRITCHARD: I have a comment about the terminology when we talk about a digital model or an analog model. The model is the math. The model is the symbolism which you've developed, the functional relationships you are going to consider to be important, in parametric form, and then the computers are simply means of solving this. In one case you simulate the functions by RC networks, and the other case you take the difference forms.

THOMANN: The distinction is really arbitrary, you solve the equation whether you use either an analog or a digital.

RATTRAY: It would be much more reasonable to talk about one-dimensional models or linear models.

CALLAWAY: Let me say one thing. I think the Bureau of the Budget has indicated that they would like to know what are the advantages of analog versus digital versus hydraulic models, which one costs more and so on.

PRITCHARD: Tell them that that's the wrong question.

O'CONNOR: Absolutely, I think there's unanimity among us on that.

PRITCHARD: I've served on n committees which dealt with that same problem, and it's just not the right question.

THOMANN: It seems to me that again we've heard several times this morning and this afternoon the notion that there are a number of models around, and in fact there are really relatively few, both from the hydrodynamic point of view and from the water quality modeling point of view. Again, there are different methods of solution, but we really only have, in the sense of a water quality model, one model that we can write down without too much difficulty, and that's a multidimensional partial differential equation with advection and dispersion, and that is about it. Now whether the solution of that equation feeds forward into another equation, such as in the BOD and DO, that's conceptually a relatively easy extension to make.

PRITCHARD: A few general comments. I would want to suggest that perhaps the requirement for the development of conceptual models adequate to treat the problems requiring answers is more important now than how one solves the mathematical formulation of the conceptual models after they're obtained. No degree of sophistication in the use of the digital or analog computers will correct deficiencies in the conceptual model. And further, I suggest that the conceptual model to be employed fit the problem requiring solution.

2. COMPUTATIONAL ASPECTS

LEENDERTSE: On the steady-state feedback thing, I wonder why you do a steady-state analysis. You can go much faster through the variable time-dependent model than you can go through the steady-state modeling. This is not the case when you have a small number, say thirty sections of the river. If you have many more than that, like if you have a two-dimensional model, you can approach the steady-state condition much faster with the time-dependent solution than inverting all the matrices. In effect, inside the matrices you generally have an iteration procedure to find the solutions. You should be very careful not to go along this line, in my opinion. You could save a lot of money on computer time. Besides, that is the way to also handle the time-dependent problem simultaneously.

THOMANN: I find that kind of hard to really grasp. What you are saying is that one can run the time-dependent general feedback model faster? To reach equilibrium?

LEENDERTSE: Yes, you can run it faster where you have more ways of arranging it. I have worked very extensively with multioperational schemes by which you do not have one representation of the finite differences, but two. I have always worked with two, but you do not necessarily have to use two. That approaches the steady-state condition much faster than just inverting matrices.

THOMANN: Yes, but we don't invert the matrices.

LEENDERTSE: Well, a relaxation technique is, in fact, a time-dependent solution technique.

THOMANN: I see.

LEENDERTSE: Also you can include the nonlinear processes. The decay operation in, let's say, BOD-DO reactions is not really linear. Even if you assume it is linear there are stops in it. You can get negative concentrations in BOD as well as in DO, so you have to stop those reactions. And that prevents you from using those types of models except only in those cases where you are also assured that you don't have anaerobic conditions.

JAWORSKI: One comment concerning feedback. I think we are going to see more parameters in water quality than BOD and DO. I think we are going to need a model that will run simultaneously, at least seven parameters. I can envision the seven as being DO, carbon, organic nitrogen, ammonia, nitrite-nitrate, phosphorus, and salinity. We will need both a one-dimensional and a two-dimensional hydrodynamic (real time) model, an expanded capability in multi-parameters with appropriate intake and feedback. I think this is the direction in which we are going, especially in the Potomac estuary. I think the capability of running at least seven parameters simultaneously, even with crude first-order systems, is something that we've got to start designing for today.

BAUMGARTNER: I don't think there's any question about that, and there doesn't seem to be anything special about, say, the Potomac. I think we are all concerned with the same thing in Puget Sound.

JAWORSKI: My point is we don't have it. If you wanted to do that today, you couldn't do it. There isn't a model that can handle it. The Orlob model can handle five.

The feedback is very important, as in the nitrogen cycle, and I want to reaffirm what Dr. Thomann stated.

PAULIK: Biologists heartily approve of the attempt to model several parameters simultaneously, because if an animal is responding, for example, to a decrease in available dissolved oxygen, the water temperature almost completely controls the response, or it may modify this by a factor of several-fold. Then you can add the other parameters in, and what you are really working with is a multi-variate response surface, and the animal is responding in a synergistic way to a combination of effects. It seems that one of the major contributions of modeling to biological interpretation of pollution is the fact that you can synthesize the animal's exposure to a variety of stresses, and you can actually integrate over, say, some migratory path for example, through different stresses in an estuary, and then interpret his total response to this combination of factors. The bookkeeping just makes this out of hand for anything but some kind of computer model. Of course, the other approach is to almost ignore the model and expose the animal directly and try to interpret the animal's response. But I think we have to work from both ends until we build some type of effective model. Perhaps we need a scheme for evolutionary modeling, so that the data we accumulate can be incorporated in the model, and monitored data be incorporated in the model. So we get a feedback here to eventually improve the model and the monitoring system.

LEENDERTSE: The results, of course, are not finished, but at the moment we are running six constituents simultaneously. These can have all the feedbacks between any one of them, and we found the numerical solutions for that. It can also be done in nonlinear processes, that is, have feedbacks between all of the constituents. So the solution methods are available. This is one of the basic questions which can be resolved right now. Then, in connection with what just was said, there have been studies made on modeling biological systems. I have here a report in front of me applied to the blood stream, physiological models, the oxygen content in the blood. Many of these programs seem to be applicable to the problems that we are faced with here in water quality studies, and we haven't touched upon them. There has been a lot of development on this in medicine, and I have a feeling that we can really step forward by using the approach which has been made in those areas and try to translate them into the water quality area.

THOMANN: Yes. I would second the notion, in answer to this tracking of multiple constituents, that I don't see any conceptual bog right now in computation. We also have a multivariable time-dependent feedback with arbitrary type of kinetics that's operating, and the problem is that we don't really know what to put into it. We don't have data yet for a lot of these areas. So I don't see any computational bog to constructing any kind of system that we want to model. I think that the problem is that sometimes we don't know what systems we want to model, we don't know which interactions are important, and we don't have data to put into them. I think the answer to Norb's question about what he doesn't have, and I believe this is your point, is that you don't have a model. The computational procedures exist.

JAWORSKI: If I could have the model tomorrow, I'd put it to use in designing next summer's program for the Annapolis Laboratory.

THOMANN: Well, let me give you an example. Jan could give you this, too. One could give you tomorrow a computational framework that had reaction kinetics in it. The instructions to the user are: you have to write what you think those reaction kinetics are; you have to write what you think the nonlinear interaction is (and in some cases we don't even know what that is yet). But the spot is there. When we all learn what to put in there then we can run some.

JAWORSKI: When I talk of seven parameters, I'm referring to running the nitrogen cycle simultaneously with the carbon and DO system, and also the salinity up to the salt water intrusion point. We could use it tomorrow. We are using the Orlob model which has five constituents running right now.

FEIGNER: To set the record straight, there is no real limitation on the number of constituents the Orlob model can handle. It happens that five are incorporated in the model, but I don't see it as a major programming effort to increase that to a larger number.

THOMANN: Oh, it very definitely can be. Yes. Where you are talking about a constituent, you are talking about consecutive reactions, but not with general nonlinear feedback. That is a different order-of-magnitude problem.

FEIGNER: [Added in proof] The basic program logic certainly does not preclude a large number of constituents being run simultaneously. The biggest problem will be to define the functional relationships between the constituents, and that can be a significant problem.

PAULIK: I was just reacting a little bit to these respiratory models. There must be at least ten of these, and there are a couple of good articles summarizing the evolution of respiratory models. Still there is tremendous disagreement between different theoreticians on the appropriate model of human respiration. And to think of the homogeneity of blood compared to the heterogeneity of water in an estuary, I think we are facing a very difficult problem, and I don't know how it can be solved by proceeding in that direction.

HARDER: I would like to point out the importance of immediate communication between the computing component of solving a problem and the interpretation of results, together with what is sometimes an intuitive readjustment of parameters, which constitute a component best supplied by the human mind. Perhaps in line with Don Harleman's suggestion of knob turning, we might imagine a situation in which one is trying to adjust a large number of parameters associated with a model so that its behavior duplicates that of a prototype for which we have field-determined data. This procedure is called verification of the model. Even if the model takes the form of a digital computer program, it might be well to have laid out in front of an operator a series of knobs that would control the value of such things as diffusion coefficients through potentiometer settings. These potentiometers would be connected through a scanning mechanism and an analog-digital converter to the digital computer program. This would bypass having to punch new holes into new cards each time there is a change and at the same time show, through the pattern of knobs, the geometry of the prototype. This would be a help to the operator, who would be trying to get solutions back within his memory span so that he would not be trying something more than once, and could enable him to more quickly achieve verification by allowing him to make his adjustments while watching the changing behavior of his model through, say, an oscilloscope display of some dependent parameter.

I have included in my chapter a description of a technique which is not yet a part of the state-of-the-art, but which I hope will soon be included in that category. This is a method I and my students at the University of California at Berkeley have called nonlinear systems identification. It's essentially a black box approach in which one attempts to define the system without knowing anything about the details. I shouldn't suggest that if you do know something about the details that you should ignore it. If you know the equations, for example, you should by all means put the equations into your analysis.

The technique will relate a series of input variables to an output variable and enable one to use the past to predict the future by a method one might call multidimensional interpolation. It has proved to be very powerful, since it does not assume that the inputs are linearly independent; and we know that most, if not all, significant problems involve nonlinear relationships. We have applied it to systems that have one or two time-dependent inputs. Each input interacts within parts of itself so that yesterday's value of an independent variable interacts with that of the day before, and input one interacts with input two at all different times in the past, and these combine in their influence on the present value of the output variable.

In those instances in which we know very little about the equations, this would be the appropriate technique because all it requires is a sufficiently long series of measurements of the system.

JAWORSKI: On this feedback system--if we're going to go feedback in our quality models (a four- or five-parameter related system), one needs a lot of time and field data to verify the various reactions. I can see a distinct advantage in a hybrid system. If we could use the cathode ray scope, and one wanted to control four reactions simultaneously, you have the capability of a direct communication with the hybrid system. This would be a tremendous advantage.

HARDER: Well, I'm not suggesting that direct communication is the monopoly of hybrid or analog systems. This can be developed for digital systems.

JAWORSKI: Say, you have a complete nitrogen cycle model in which there is linkage in the organic nitrogen to ammonia to nitrite to nitrate and back to organic. You have about four or five reaction rates to verify or adjust which govern the concentration of a given species at a given time.

HARDER: What you mean is that a particular reaction rate depends upon three or four other dependent variables and the reaction rate of each of these variables depends upon it and the others, so that they are all coupled, and they cycle and in a sense there is a feedback. But when you simulate such a system, you do it by carrying out an integration in time of all dependent variables at the same time. And at each step you pick up the value of the others, insert that into an equation, and find the derivative of each one of them and carry it forward one step. I think that's the modeling technique, and that, I believe, is what you mean by feedback, and it's certainly a very powerful method. In particular, it brings out your ignorance of some of the terms.

JAWORSKI: Many terms are unknown to us. Moreover, there is often quite some time elapsed between data collection and model verification. This time could be anywhere from weeks to a year until you have adjusted and readjusted the coefficients to your satisfaction. I'd like to reduce some of that time and we may be able to do this with the use of the hybrid system.

HARDER: Well, that's where the immediate back-and-forth communication between the computer and the operator is very, very important. And if you can effect that with some digital computer oriented equipment, it would do just as well as if it were an analog computer oriented equipment. I think the important thing is the rapid communication. The particular machinery, whether it's analog or digital, is not so important.

I'd repeat though the advantage that you have with analog equipment, and that is essentially you don't have any continuing operating costs. And that gives you the kind of comfort of knowing that you can waste a little time without going over the budget. The digital computers are dreadfully expensive if you have to go through many, many, many steps to achieve verification.

PAULIK: There are some systems like DYNAMO and others that are used by economists. I don't know if you've looked at any of these and have any opinions on them. They're simple first-order linear difference equations, but they can handle thousands of equations.

HARDER: Yes. They're coupled first-order differential equations, I'm pretty sure. The trouble is that we don't know the coefficients that go into the terms. Solving the equations is not the problem.

3. DATA COLLECTION AND VERIFICATION

JAWORSKI: BOD-DO modeling is something that we can usually do quickly, but I think when you start looking at nutrients, phytoplankton populations, zooplankton populations, you're talking about quantum jumps in numbers of field data. One thing we have to impress upon our administrators is that we are talking large populations of data required to verify our more complex modeling.

WASTLER: It's all very well to say this from a philosophical standpoint, but when you get down to it, where do you sample, when, with what degree of accuracy and how are you going to use it? There are the questions that come flying right back at us every time we start talking about sampling programs, data collection, and mathematical models. But this is not the kind of thing that you give to an administrator. You give him some guidelines by which he can decide what level of resources have to be committed to produce the results.

CALLAWAY: The verification process again. Doesn't that still boil down or come round-circle to verification not being so much a problem of not having the right data at the right time, but not having the right information on coefficients?

THOMANN: Yes. We're always interested in returning to some kind of first principles. In this context of reducing numbers of knobs, certainly.

WASTLER: Would there be any way to explicitly state how much data would be needed for reasonable verification?

THOMANN: Well, I think that bears heavily on the problem context, what kind of problem are we actually attempting to solve in a given context. If, for example, we are concerned about hour-to-hour fluctuations where some of these real time models are concerned, then that's one type of sampling program. If, however, we're interested in mean value type programs, such as the overall effect of a treatment plant on a particular estuary, that's a different kind of sampling program.

WASTLER: I would like to see some comment possibly on the specific kinds of studies and information needed to fill in some of these holes. One of the things we're working toward right now is development of essentially a coastal monitoring system, which hopefully is not going to be just a means of going out and collecting numbers. But we would like to develop it within the concept of the kinds of information that are actually needed to solve some of these problems. So any specific comments any of you gentlemen would have regarding this kind of information would be greatly appreciated, particularly if we can use your names in vain as having recommended them.

DOBBINS: In the estuaries themselves there's no question that nitrogen effects are extremely important. We know that every gram of nitrogen requires maybe four grams of oxygen to oxidize it. And I know that this is true in some of the young freshwater streams away from the estuaries themselves where there are cases that the quality of the stream is actually deteriorated by building a secondary treatment plant. There are small tributaries of larger rivers with small primary treatment plants located on them which, say, has two days hold time to reach a safe haven in the big river. The stream will be somewhat degraded. But then you build, let's say, an activated sludge plant on this stream and you turn out an effluent ripe for nitrification, then the nitrogenous oxygen demand is going to be exerted in those two days, and the stream will actually be probably worse off then it was before you put in the plant.

I think the whole biological interaction between bacteria and algae is very complicated and deserves a lot of study. This falls back to biologists. These things are complicated by the fact that we have many fundamental periods involved. First, there is the tidal period, twenty-four-and-a-half hours, then you have the diurnal period which is the period that most of the inputs, the algae effects, follow, and over a long period of time you have the seasonal effects. There's no such thing as a true equilibrium ever being reached.

WASTLER: Well, one of the apparent things was that on a routine monitoring basis it would of course be impossible to measure all possible parameters. One of the things that we're concerned about, recognizing that to pin down a number of these interactions will require intensive study in specific areas, is what kinds of information could be collected on a routine basis which would support this kind of investigation?

PRITCHARD: I'm not sure you're at the stage of saying just "routine" sampling. We need to know more fundamental facts about the response of the ecological system to water quality. For instance, one finds quite a difference between the effects of nitrogen in systems of fresh water than in the estuary proper where there's salt water. We can find great differences in the character of the primary and secondary food chains in the upper Chesapeake Bay over periods of time. Every spring the major nitrogen source is the input from the river Susquehanna, and during the spring runoff the nitrate concentration runs around 70 microgram atoms per liter or higher. By the first of June, the concentration of nitrogen throughout the upper sixty miles of the Bay and all the tributaries is about 40 microgram atoms per liter. By the end of summer and beginning of autumn that's down to four-tenths of a microgram atom per liter. That difference is all going into the bottom in the form of unoxidized organic material which does not return. We never go anaerobic except in very local regions. And the supply of nitrogen is renewed every year and chewed up every year, and there's not any great difference between a hundred-fold variation of nitrogen concentration. But we do see significant differences in the estuary with respect to the phosphate. Now, maybe it's not the phosphate but something that goes along with it, other organic stimulants or something else. But it's quite a different thing than in the freshwater system where the nitrification appears to be an important part of the system. My point being that in some systems you might say that ten microgram atoms per liter of nitrogen is too much, but here we've got a system that responds not essentially any differently between when the nitrates (and in this case this is most of the nitrogen) in dissolved form is 40 microgram atoms per liter in one case and down to .4 in the other, and still functions in essentially the same way.

One very fundamental question, for instance. We have been trying to run the nutrient balance in the upper Chesapeake Bay. There is in fact a sizable amount of nitrogen and phosphorous produced by the Baltimore treatment plant. We don't see it in the upper Bay. Why? Well, we think we know why we don't see the phosphorous. But we have no simple explanation for nitrogen which we also don't see, and we should. Now there's some fundamental thing happening to the nitrogen that has been put out of the sewage treatment plant.

THOMANN: Did you try running a nitrogen model? You know, trying to track the nitrogen and see where it is going?

PRITCHARD: We are trying, but it is very difficult.

RATTRAY: Another thought about monitoring, a partial answer. If you can get some measurements that give a measure of rates. I've been jogged again by the people worrying about nonconservative reactions or properties which have rates of reaction or exchange associated with them. I keep coming back and saying that the equilibrium salinity distribution is not a measure of the rate of salt flux and it is the rate of movement of salt through this cross section, which is the rate of movement of water through it at different levels, that will have a much more marked effect on the time-varying distribution where a rate is involved, which has a time clock built into it. Something goes by and is decaying as it moves by. Its distribution would be very much affected by the rates that things are going on, the rates of movement of water, whereas the salinity, which doesn't have that time clock built in, is not very hard to determine. There would be a big difference here. Not only do you have to worry about what the rates are from biological and chemical factors, but the hydrodynamic models which will have to go along with it will, I think, be necessarily more complicated, as you have to worry about the rates of things as opposed to what's in equilibrium.

PAULIK: In a way it seems the total objective of the monitoring system should be considered. In solving a number of agriculture problems when we set up the land grant colleges to work on these problems, we certainly didn't have the advanced physiological and chemical knowledge that we have now, and we did this empirically. The monitoring systems in particular areas are going to be tied into key species, which are desired species in that area and have to be protected, and these will be simple bioassay systems or continuous bioassays. Here you might be concerned with sampling problems to make sure that you have a sort of consumer, or vendor, and purchaser risk as in selling any type of material, but you are concerned with the basic problem of sampling some key species to make sure that this species is protected. And until you define all your objectives of a particular monitoring system, it seems very difficult to set any general set of rules which will establish the basic criteria for a monitoring system you can employ in any estuary in the country.

WASTLER: The basic purpose behind any monitoring system run by FWQA is to maintain surveillance of water quality in order to determine where water quality degradation exists so the proper mechanisms can be taken to combat it.

PAULIK: Well, this brings in the problem of defining what is degradation of water quality. You might be concerned with the striped bass in San Francisco Harbor, which have a critical time in their life when they are dependent upon adequate spawning grounds and the eggs have to be protected during a certain, very specific period, whereas in another estuary you might have a very different set of problems. It seems these problems are the ones that define what you mean by high pollution and degradation.

WASTLER: Each system is in some degree different from all others, and the scope of the monitoring system, including the timing and parameters measured, has to be related to the problems and characteristics of that system. But what I am driving at here is, in the process of carrying out this general objective, we have to take certain measurements on a certain time scale. I am trying to get an idea if in carrying out this objective we can, say, modify it slightly to contribute toward the basic effort of developing predictive models and understanding the interactions. I would not like to give the idea that such a monitoring system would be set up purely for developing information for mathematical modeling or any other kind of modeling. But I have a feeling that it can contribute significantly to the data base which would be useful in developing such models.

PAULIK: It seems like it should go hand-in-hand with modeling so that these short-term forecasts can continually be made on the basis of the data you're collecting. You could somehow integrate this with the type of fragmentary results which are available in biology now. All types of physiological studies are being put together in modeling efforts, or at least in estuarine problems. In trying to make forecasts, your data could very nicely pull into models based on synthesis of some of the physiological work that is being done.

RATTRAY: At this stage it seems like a few, easily identifiable quantities which don't interact very much, only one or two interactions so that the system which you consider is simple, might be very useful. They may not be the ones important to water quality but they might be the ones very useful in measuring and determining what is going on in the system.

WASTLER: That's quite true. And once you're out there collecting samples or you have established an automatic monitoring set-up to do it, it's sometimes quite simple just to add another parameter which would be useful for a specific purpose. We would certainly be happy to hear of any specific parameters that might be useful. Not necessarily right now, but any time they might occur. I think Bob, in particular, understands the problems.

THOMANN: I think the problem there is that some of the variables that we would eventually ask you to take a look at would be more difficult to get than you may care to incorporate into a routine monitoring program.

WASTLER: This is certainly true, but...

THOMANN: But you would like to know them anyway.

WASTLER: We would like to know them anyway. As you very well know, sometimes if you can do some advance planning, you can take care of such things over a period of two or three years.

PAULIK: Well, it seems important, just as a general rule, to somehow simultaneously observe the reactions of the higher organisms, zooplanktons for example and some of the fishes too, at the same time you are taking the chemical and physical measurements. This is the one problem that continually plagues biologists trying to build models, that we have grab samples or samples taken at infrequent intervals or when the weather is favorable, and we try to find physical and chemical measurements taken at the same time. It's very tough to get an integrated series of biological and other measurements to interpret the biological measurements.

I have a couple of comments. One on Chapter III where some of the philosophy of model verification is put forth. I wondered if some of this could be tightened up a little, and perhaps some sampling strategies suggested. There seem to be a number of problems here. How do you lay out a sampling grid? What's the frequency at which you collect samples? What are the problems of verifying the model using grab samples versus some sort of continuous monitoring system? What are the precision requirements on the individual parameters that you're measuring? You can develop a theory of propagation of errors in which you can look at the precision with which you measure some elementary variables and then combine these in various functions to build up your final random variable that you'd like to plug into the model. And I think that Dr. Thomann has laid out some of the problems here, but I wonder if there is any theory or any references that would be of help to people building models on how they can set up sampling programs to verify the model or to test model validity. I don't think there are any general statistical techniques. Perhaps some of the time series techniques give you some idea of the model validity over time. But I think that the problem, that at least occurs to me, is how do you begin to sample in terms of the statistical theory of sampling, and how do you design the combination of, say, different treatment conditions you'd like to look at, to actually collect the data you need to verify the model?

THOMANN: Yes, well taken. I think there is some information and some work that has been done on the application of some statistical analysis to the construction of various types of sampling programs. I don't know of any rigorous, statistical sampling theory framework that has been developed for water quality monitoring as yet. This is certainly an area that we want to feel out for future work.

CALLAWAY: I got the feeling, though, while you were talking, that you looked down on statistical tests because there wasn't enough data available to justify them. This just means that you want to generate more field data rather than that statistical tests aren't good enough, right?

THOMANN: I don't think it's a question of looking down on statistical verification. I think that the point was that in many actual situations, the amount of data that's available for problem verification wouldn't warrant it. What we do have occasionally may very well reflect highly localized situations. For example, a number of models we've talked about so far are difference models, representing finite lengths along an estuary that are essentially assumed to be completely mixed. What we need to actually verify is some good data that we can be reasonably assured is representative of the average over that entire length and over time. We often don't have that and that was the point. In other words, we occasionally see comments like why not grind right into the modeling close up a type of optimization procedure that takes the model output and starts iterating around observed data until you get a best fit between model and observed data. In many situations, I don't think it's worth it. There are situations where it may be.

WASTLER: Would it be possible to lay this out explicitly? What would be your criteria for a suitable data base for a given kind of model? Is seven points of data enough taken over a year or do you need twenty million?

THOMANN: Well, I think at this state there probably hasn't been really enough done on that whole aspect. But I don't think there are any specific guidelines, rigorous quantitative criteria that one could spout at this stage. There are certain things that can be said. If you know, for example, underlying distributions, probability density functions, and you have some idea of the confidence level that you want to achieve for a specific type of problem context, then there are some general statistical guidelines that can be used to generate the numbers of samples required to achieve that specific objective with a certain degree of confidence. I don't know how useful that is at this stage in the estuarine quality area.

WASTLER: Well, it would have a basic relationship to how you would go about setting up a sampling program.

THOMANN: My own experience has been that it helps just very, very generally. But what usually constrains it? What kind of program you can mount within a given time period. You know there are so many other extraneous variables that come to play in mounting a sampling program that rigorous statistical frameworks may not give you the kind of information you need. Budgets, sampling programs, lab facilities, how many people you have to put up. Those tend to be almost overriding considerations in most of these sampling programs. Now if you are posing the question: suppose there were absolutely no constraints. Then that's a different situation.

WASTLER: Well, agreed that the budgetary-personnel factors are overriding. But there is little point in, say, spending a half million dollars to develop a highly sophisticated mathematical model when you don't have the data base to verify it. And it's this kind of criterion that I'm looking for some guidance on. As you know, this is one of the things we have to face everyday.

BAUMGARTNER: I think those things you mentioned, Bob, as constraints are not things which are foreign to people who have to design sampling programs. And I think there are pretty well-defined and perhaps rigorous, in their mind, techniques for how you get the best sampling program for these constraints. So I don't think it's unrigorous, or I don't think we can say that kind of rigorous analysis is not available.

THOMANN: Well, by rigorous analysis, I mean some kind of analytical framework.

BAUMGARTNER: I do, too.

THOMANN: No. I haven't seen it. Seriously, I don't know where it is. Isn't that exactly what you're asking?

BAUMGARTNER: No. I'm talking about sampling programs as designed by statisticians who are working with surveys. Books like Cochran and Cox for one, I recall. Maybe you know of this one, Jerry. And I think the framework is pretty rigorous.

PAULIK: Well, the framework there is very rigorous. You can define a frame, a sampling frame, and you also know what your population is. You certainly have certain clear objectives. Here, a lot of the problems to me seem to be very fuzzy. Approaching a problem in an estuary, I as a biologist would start looking for the key species, looking for the life histories and their interactions with other animals. I would eventually get down to how I thought the environment affected these species, instead of starting with the very detailed modeling of the environment and building up to the species. I'm not at all sure how you begin to sample in this context. That's one of the reasons I'm partly asking for information and addressing the question to Bob. I think there is very good statistical sampling theory in certain areas, for certain objectives, and I'm not clear, I guess, as to what the total objectives of estuarine modeling are. That's my problem.

THOMANN: If you ask questions like: how many samples would I have to take to be 95% confident that a particular value is within plus or minus five percent of something. That we can do without any sweat at all. And that's done very often in collecting waste effluent samples, to some extent water quality samples. My own experience is that once you do that, it's a nice number, one looks at it, and eventually what happens is that an overriding consideration is what you can do within a specific time frame. But if you phrase the question rigorously then there's a rigorous framework. It turns out some of those sampling requirements go up nonlinearly, as, for example, the variance of the process. There's another thing. We don't know very much about the variances of some of these water quality constituents, and very little about their statistical behaviors. We can use some non-parametric statistics, but that doesn't bring us very far either. We've got a lot more, no doubt, to do. And because those sampling requirements go up nonlinearly, it becomes important. But I don't think we have any rigorous approach. We don't. There may be other fields that have it.

BAUMGARTNER: I have the feeling that many of the people who are working in this area don't even appreciate that this kind of statistical test is available.

WASTLER: This relates back to Dr. Harleman's comments this morning, with regard to the different time scales. Obviously if you are going to talk about tidal fluctuations, samples taken every week are not going to help you very much. Likewise, if you're talking about annual trends, there's hardly any point in going out and measuring every thirty seconds. I was looking for some general guidelines or directions.

DOBBINS: I think you put your finger on something there. I think if you have so many dollars to spend on sampling, and you have so many estuaries to sample, it's more efficient to concentrate, studying each estuary over a relatively short period of time, very intense sampling patterns with short time intervals, then move to the next one, rather than study them all at the same time on a very coarse network.

RATTRAY: I would certainly second that. I've never seen, and maybe nobody has seen, an over-sampled estuary.

DOBBINS: If you would sometime just move in, maybe one month, and really concentrate sampling and get the pulse of this one, and then move to the next one. But taking a sample once a week in all ten of them isn't going to give you anywhere near as much information as taking ten samples in one.

HARDER: I might bring out something which is fairly obvious, and pardon me if I am elucidating the obvious, and that is if you know the rate at which a certain variable is changing in nature, that automatically gives you the time scale at which you ought to sample. Certainly you should sample no less frequently than two times within the period of the highest frequency at which something changes or the frequency at which you think it is important to record things. And the same thing relates to distance. You can define a spatial frequency, if you like, and you ought to sample at least twice every time you go through a cycle of spatial variability. These things then would give you a guide. Now certainly if you are going to construct a model the sampling ought to be reasonably well related to the nodes at which you expect to make the computation, which is a way of feeding back from the model to the sampling program.

FITZGERALD: We continually get this question. We're going out and sample this estuary for two weeks. How many samples should we take? How should we take them? How often should we sample? This is continually asked on an operational level. Normally we just say once every half hour every hundred feet, since the majority of them aren't going to do it anyway. But I don't really know if there is a clear answer to deal with this point.

DOBBINS: I think you have to define the objectives of your central program. If it's merely a monitoring program to determine what the conditions are over long periods of time, then use a coarse network over a large area. But if the objective is to determine parameters which will enable us to improve the mathematical models, then you've got to do intensive sampling.

* * *

THOMANN: I think in the final analysis a lot of these questions, at least in my own mind, can be answered by actually playing the forecasting game itself, and we haven't done this very often at all in any of this water quality work, or in fact not really in any of the hydrodynamic modeling either. By forecasting I mean that you know everything up to time t. Given that information, what happens at $t + \Delta t$?

DOBBINS: This is okay if the inputs to a system change after time t, but if the inputs remain the same then we're still fitting the same curve. This is what bothers me about these long-time-averaged models. We look at DO in an estuary. It is a fairly simple sag curve, oxygen declines then it rises again. The old Streeter-Phelps equation gives you a functional shape like that, and you can fit the Streeter-Phelps equation with these very simple inputs to many of these sags. Then we go back and we become aware of more and more of the inputs. We include those in the equations. We still get a good fit. We now have to go back to adjust the first values of the coefficients we had. As we keep adding more and more inputs and feedbacks into the system, we're still getting a good fit. We're getting a good fit with all these models. So therefore it leaves you with the agonizing doubt, does the latest one still have all the inputs of concern?

THOMANN: And the answer is probably: no.

DOBBINS: And the answer's probably no. And verification, in my mind, is really curve-fitting. It's a model to fit a curve, to put a functional description to a curve that you can measure in the field. But the only true verification it seems to me to be to determine if, when you remove some of the inputs, will the effects of this removal will be borne out by your equations, the predictive equations. I don't know of any case where this has been really done. The test of all these is to come.

THOMANN: Well, I think I disagree. I generally agree with you on several points, but I think I disagree that verification for the kinds of models we're talking about here is nothing more than passing functional relationships through a set of data. After all, one could take a plot of data as a function of x and do some regression analysis on it and then fit some function. The point of departure here of these models is some kind of fundamental physical phenomenon.

DOBBINS: Oh, I agree.

THOMANN: Now, at any point in time, we may not appreciate the entire depth of what that physical phenomenon involves, hence the old Streeter-Phelps sat around forty years and really wasn't dealt with much beyond that. So I don't see it just as passing functional relationships through data, because we could do that with regression.

DOBBINS: All I'm saying is that we should be very cautious about believing that we've got the final model.

PAULIK: Well, you don't kid yourself if you're just estimating, say, the coefficients in a nonlinear model. If you have a simple food chain model, you've got data from radioactive tracers moving through the food chain, and then try to generate the same data from a simulation model and where you know the underlying structure put some error terms on it, and then try to employ statistical theory to estimate the constants, you loose total faith in your original model, your original concept of how the system worked. I have the feeling that some of these models may be of the same type, that we have a whole system of constants, and the constants are very difficult to estimate statistically. I know of no standard theory for how to generate an adequate sample to verify the model. If you have a number of different segments for example in a stream, and you are using your model, you might ask the question: how many of these segments have to be sampled to give some sort of reliable estimate of the coefficients in the model? Is it possible to make that type of judgment?

DOBBINS: The objective of all this, as I see it, is to help us come up with engineering judgments as to what we have to do, and what inputs to the system do we have to remove in order to restore these estuaries to an acceptable form or level.

THOMANN: I think that's true, and, to me anyway, these models have been very useful. I certainly agree that we can't be overconfident. Now the state of knowledge of what's happening is increasing very rapidly and we can't really think at any one stage that we've got the whole thing wrapped up. But I found these particularly useful for several reasons. It helps to set a kind of framework for decision makers that didn't exist in the past. Order of magnitude responses, for questions like the New York Harbor situation where after secondary treatment is installed, what is the general level of improvement you could expect, even given these crude models. Well, it turns out a couple of tenths of milligram per liter dissolved oxygen. Now that, in and of itself, is the kind of information that didn't exist five or ten years ago, and is very useful toward the decision-making process. Now, if you are in fact going to go out now and try to sample the system to detect that two-tenths of a milligram per liter of DO increase in the face of background noise, that requires some rigorous design in how many samples you have to take, and so on.

WASTLER: The question is, do you believe that result?

THOMANN: Well, I believe it's not two. I believe it's not off by more than an order of magnitude. That's the point.

EDINGER: Isn't there also a data requirement for observations we need to determine how to design the model? For instance, I don't think we're at the stage yet where we can say that we can predict for n interactions every possible combination of thing that could go on, and go out in the field and apply it and come up with anything. Take, for instance, your work a couple of years ago on phosphate cycling where you suddenly discovered just from rough field data that you were turning over quantities of phosphate every two or three days. I don't think it would show up in the model until you explicitly designed it in. And yet it is things like this that we are suddenly discovering that makes a water quality problem what it is. The same thing I think is true with the problem of the nitrogen cycle in a body of water. For instance, as I understand it now, and this is out of my field, apparently there is some concern over nitrogen in the Delaware being very temperature sensitive, that below certain temperatures there is very little oxygen response to it. Would this have been built in _a priori_, or are we still in the stage yet that we have to intuit these things out and get the data to discover that they are going on?

THOMANN: Well, in a lot of cases, yes, it is very temperature dependent. The question is: five years ago, ten years ago, it probably wouldn't have been there because it simply didn't occur to us. But I think the point here is that I don't see us building models in a vacuum. The data that we get from the field shapes the models, and the models help shape how we collect data, a continual type of interaction between data collection and modeling and data collection again. We can't hope to model something we've never even observed.

4. PREPARED REMARKS

4.1 DISCUSSION by George H. Ward

Dr. Pritchard has rightly pointed out that the kinds of estuarine water quality problems that you face, the decisions to be made, and hence the kinds of models you require depend to an enormous extent upon where you are. This observation can hardly be overemphasized. From a practical standpoint, there is no universal estuarine model: in an estuary, the pertinent water quality problems must be determined and the relevant processes identified in order that meaningful and utilitarian models be employed. Conversely, the limitations of existing estuarine models should be similarly considered, their underlying assumptions and the approximations made in their development, so that they are not applied to a situation for which they are not strictly valid.

Now this merely restates some sentiments that have already been expressed by several of the people in this study. But it does serve to underscore, however, the fact that the bulk of the state-of-the-art of estuarine modeling, at least as represented in this report, is concerned with coastal plain estuaries of the type extant on the north Atlantic coastline of the United States. While it is true that models have been developed for systems such as Jamaica Bay on the east coast and San Francisco Bay on the west, which require a two-dimensional representation, and while it is true that many of the model formulations are of more general applicability, nonetheless most of the work in developing and applying estuarine models has been directed toward our northeast coast estuaries, as this is where the earliest pollution problems have occurred. But in the context of this report, we must point out that there are other kinds of estuaries and other kinds of problems which also require study. I am thinking in particular of the Gulf Coast estuaries which have been, undeservingly, somewhat slipped over in this report.

By "Gulf Coast estuaries" I mean to include those bays and sounds contiguous to the Gulf of Mexico and lying along the arc of coastline extending from behind the Florida Keys around to Padre Island on the Texas coast, excluding, however, the estuary of the Mississippi. Typically, these estuaries are broad and shallow with an average surface area of some 500 square miles and a mean depth of ten feet, and are fed by multiple inflows around their periphery. Many of these estuaries are nearly isolated from the Gulf by barrier island paralleling the shore. These estuaries are highly productive and are extremely important to the commercial fishing industries in the Gulf. (See Gunter 1967 and Odum 1967 for general features of these estuaries.)

Hydrodynamically, these estuaries present something of a different problem than such geomorphological cousins as San Francisco Bay. The influence of tides, for example, is much less important. The tidal range in the Gulf of Mexico varies from a maximum of just over two feet to a minimum of a couple of inches. The influence of this feeble tide is further dampened by the semienclosed, shallow physiography of the estuary. Winds, on the other hand, are a dominating factor in these estuaries, governing both the advective and diffusive transports through driven currents and wind waves (Collier and Hedgpeth 1950, Gunter 1967); models capable of predicting these phenomena range from primitive to nonexistent. The dynamic influence of the horizontal salinity gradient (see Chapter II) may be especially significant in many of these estuaries as well. The intrinsic transience of these systems is a difficulty in itself, their response to changing meteorological conditions, surges of inflow alternated with periods of relative drought, and so on.

As a general rule, dissolved oxygen is not yet a problem in Gulf Coast estuaries--there are local exceptions of course, the Houston Ship Channel for one, nor can we be sure how long this situation will last. However, there are other quality problems, many of which are becoming critical. These include the introduction of types of wastes which although constituting a "low-level stress" exert profound influences upon the ecology, bacterial contamination of shellfish areas, the effects of dredging and channeling, accumulation of nutrients, and the upstream impoundment or diversion of freshwater inflow. (See Wohlschlag and Copeland 1970, Chapman 1968, and Copeland 1966 for a discussion of these and related problems.) Thermal discharges can be a problem, but here I must disagree with the statement (Chapter IX, Section 1) that when cooling becomes a constraint the discharge is "too big" for the estuary. Due to the extreme shallowness of these estuaries, the effective dilution is considerably less than would be expected in, say, an east coast estuary; consequently the plume area is larger and loss to the atmosphere becomes a significant part of the heat balance requiring explicit incorporation. But this in itself does not mean the discharge is too big for the estuary, for both the surface area of the estuary and the discharge location must be considered in assessing the effects of the discharge. For example, in Galveston Bay a typical discharge into five-foot water produces an area 1°F above ambient on the order of 500 acres. This, however, is only slightly over one-tenth of one percent of the total surface area of the Bay. The critical question then becomes whether that area affects the habitat, breeding or nursery areas of any temperature-sensitive species, or encroaches on the migratory paths of such species.

In sum, the Gulf Coast estuaries present somewhat different problems, hydrodynamically and quality-wise, than are encountered on the east coast, many of which require fundamental research. Because of the singular fertility and complexity of these estuaries, a considerable effort may be necessary to clarify the links between the activities of man, water quality parameters, and the natural ecosystems. Furthermore, because of their hydrographic characteristics, they exhibit a faster response to man's activities than other estuaries. This aspect, particularly with regard to the industrialization of the Texas coast, has motivated the suggestion that they be considered a paradigm for the management of man-nature systems (Odum 1967). Clearly, the use of models is an essential part of this.

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4.2 DISCUSSION by Richard J. Callaway

Some reports don't need summarizing--this one does. Since no one else has volunteered to put things right I'd like to take at least a superficial whack at putting it in perspective. (In addition, I don't think the authors or reviewers are detached enough to do it themselves.)

Not too many years ago it wasn't unusual for oceanographers to be highly proficient and productive in many aspects of their science. For instance, G. A. Riley (admittedly, not your typical oceanographer) probed the physical, chemical and biological processes of the ocean as well as being the first to employ Lotka-Volterra prey-predator relationships cum nutrients to model these processes. In the past few years the oceanography camp has gone the way of most "new" sciences from the era of the generalist to that of the specialist and, for better or worse, rather esoteric niches are being created at a great rate. It seems to me that estuary-type sanitary or civil engineers have also arrived at a departure point, except instead of becoming narrow specialists they can become more diverse, at least for a while before things get too complicated, sophisticated and unmanageable for one man as it did for the oceanographers. Until that time arrives (and some would insist it already has) there are opportunities for the versatile to do many interesting and useful things covering a broad range of subjects. In this pioneering sense, the material covered in this report is still manageable although perhaps some pages are harder to read than they really need to be.

What this state-of-the-art report is all about is solving the advection-diffusion equation with source and sink terms,

$$\frac{\partial s}{\partial t} + u\,\frac{\partial s}{\partial x} + v\,\frac{\partial s}{\partial y} + w\,\frac{\partial s}{\partial z} - \left[\frac{\partial}{\partial x}\left(K_x\,\frac{\partial s}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_y\,\frac{\partial s}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_z\,\frac{\partial s}{\partial z}\right)\right] = \Sigma S$$

The equation might be viewed as consisting of hydrodynamic terms on the left-hand side and pollution terms on the right. In the past it has been the practice to consider that the heart of the problem lay on the right-hand side of the equation. For a long time in sanitary engineering the right-hand side has usually consisted of BOD and DO terms only; actually sanitary engineers have been making an honest living for about 45 years by employing first-order reaction rates for BOD as a carbonaceous sink. More and more, but somewhat reluctantly, they have begun to consider (and use) other sources and sinks and to employ Michaelis-Menten kinetics. Much of the discussion revolves around how to get at the velocity and diffusion terms, especially when nonsteady-state conditions prevail. There is a tendency to try and get around the u and K terms by fair means or foul, such as by averaging them out of existence or expressing them functionally. While the right-hand-side people are bedevilled by rate constants, the left-hand-siders agonize over isotropy, and von Neumann conditions (after all, if he was interested in error analysis then the problem isn't likely to be trivial and, plain to see in Leendertse's paper, it isn't). The position of the practicing engineer is that he must be concerned with both sides and really can't devote his life to fretting about any one of the K's or S's in particular.

In a way, the discussions and papers presented here seem to accentuate Levins' (1966) ideas that mathematical models sacrifice either generality or realism or precision at the expense of the remaining two quantities. For instance, box models on the one hand are abhorred by some because one might unknowingly leave out something; in effect they may be too general. On the other hand the box model has been, and still is, quite successful in investigating systems that cannot be quasi-realistically described any other way either because of the size of the system studied (see, e.g., Broecker and Li 1970), or because the hydrodynamics are largely unknown. It also seems a bit silly to argue the precision of one's guess on the magnitude of exchange processes. The one-dimensional estuary model, whether employing tidally averaged or real-time concepts, also has its reluctant admirers and has been highly useful in spite of the fact that no real one-dimensional systems exist. It is hoped that the newer, hydrodynamically founded, two- and three-dimensional models will be tractable enough to encourage their routine use while still being developed.

In the case of (electronic) analog and hybrid modeling, the state-of-the-art appraisal seems to be that the analog peaked out in usefulness a long time ago. The almost immediate visual display of results that was once the sole property of analog machines can be handled, although not routinely, by CRT devices which are now standard peripheral equipment on time-sharing digital computer systems. (There is always a danger that those who get good enough to use these devices routinely will become more enamoured of programming and the computer system than the engineering problem.)

The feeling on physical hydraulic models ranges from viewing them as gigantic toys to seeing them as having great potential in carefully selected pollution problems. As in all things, there is a danger in misuse or misapplication. For instance, obtaining diffusion coefficients from the hydraulic model in order to insert them in a mathematical model is not the best of ideas if only because the hydraulic model is not scaled to reproduce eddy diffusion. Likewise, proper scaling of the processes governing the distribution of nonconservative substances, such as those controlled by biological phenomena, doesn't appear to be all that easy. Since there are better ways to estimate rate coefficients such efforts would be better spent elsewhere. The hydraulic model is here to stay, however, because it still is the best method in which to study channel modifications (for which it is chiefly intended, at least by the Corps of Engineers).

The hydrodynamicists are in the almost enviable position of knowing a good deal about what they don't know: i.e., how to relate something measureable to something that has long defied routine field measurement and correlation, namely vertical and lateral viscosity and diffusion terms. Functional relationships for vertical eddy terms and velocity profiles can be expressed for a variety of laboratory plume conditions; when exposed to the cruel light of even the well-mixed estuary they are sometimes useful as a guide as to how nice things could be. (One is reminded of the probably apocryphal story of Einstein's advice to his son, a distinguished fluid dynamicist, to avoid hydrodynamics on pain of horrible boundary conditions.)

When it becomes necessary to include the effect of feedback on the computation of motion or concentration, additional problems arise. Such events are handled routinely through coupled differential equations. We are bound to see more and more of these with the systems of equations necessary to relate the nutrients-phytoplankton-zooplankton on up the scale to the highest user. One should not lose sight of the problem because of imagined complexities in solutions. For instance, the five equations Dr. Paulik showed can be solved with about two dozen program statements if the coefficients are known. The real problem is again getting at the coefficients, only this time there are fourteen of them and they are all maddeningly elusive and uncertain. (Add to this that what Paulik has shown is the simple case.)

The report has accentuated a recurring theme in the history of the science and engineering game: what were once thought to be solved problems are becoming unsolved with frustrating rapidity. It behooves the engineer to make use of the best tools available and to make sure he trades in the old ones, an old saw to be sure but especially relevant when he is responsible for making recommendations on million-dollar investments in treatment plants and disposal schemes. So now let us minimize our uncertainties and press forward into the Age of the Great Coefficient Hunt.

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4.3 SOME PROJECTIONS FOR THE IMMEDIATE FUTURE by Jan J. Leendertse

The contributions in this volume show evidence of historical developments and approaches used by different investigators in the engineering and the scientific disciplines, who are now tackling the problem of establishing cause and effect relations in estuaries. From these developments certain projections can be made for the use and power of mathematical models in the near future.

The development of models for estuarine processes is difficult, complex, and, in addition, costly. Generally speaking, models are made for the investigation of results of certain actions, or for the evaluation of alternate approaches concerning fluid waste disposal or engineering construction in the estuary or the adjacent watershed. The purpose of the investigation provides the analyst with tentative answers to two basic questions always raised in modeling: what problem will the model help to solve and what is the accuracy required. The answers to these questions will guide the investigator in the selection of the important processes which have to be modeled.

The contributions in this report give evidence that even with modest accuracy, complex models are required. Modeling of estuarine phenomena is a major undertaking which is generally underestimated. Therefore, it is warranted to analyze the model development effort itself. The major steps are shown in the figure with the main stream of the processes indicated. The data is placed at the top for a good reason. No modeling effort can be started without data as such data give the indication of the major processes involved. The figure is self-explanatory, except possibly the connection between conception and finite-difference models.

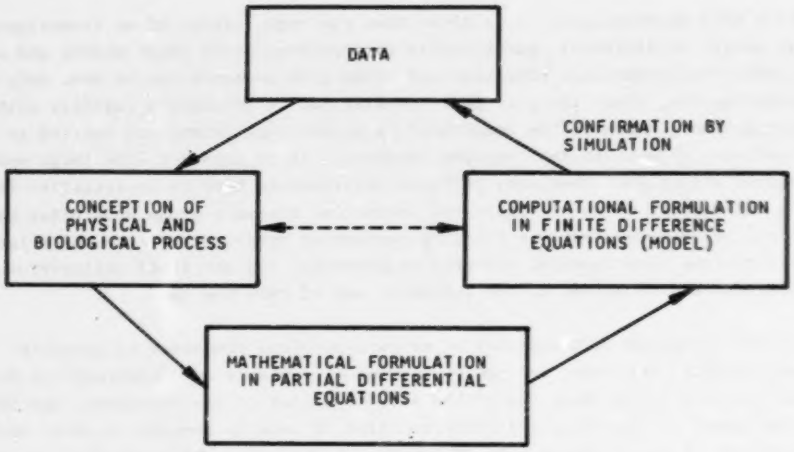
DATA
CONFIRMATION BY SIMULATION
CONCEPTION OF PHYSICAL AND BIOLOGICAL PROCESS
COMPUTATIONAL FORMULATION IN FINITE DIFFERENCE EQUATIONS (MODEL)
MATHEMATICAL FORMULATION IN PARTIAL DIFFERENTIAL EQUATIONS

Fig. 9.1 Construction of estuary models.

Conception and the resulting mathematical formulation are often inherited from the pre-computer era. In those days, the only hope for solution of the derived equation was an expansion of products of the dependent variables followed by a simplification so that analytical methods could be used. At present other formulations are required which are more suitable for the subsequently derived finite-difference equations. As indicated, not only approximations to the partial differential equations can be made but also conservation of properties with a physical meaning can be achieved.

The loop in the steps of the development shown in this figure is closed by verification of the model using actual data. It may be necessary to iterate through this development several times. In the verification of the model, we interface with the technology of data collection and with the aspects of data representation, both of vital importance for a successful investigation. Digital records from field explorations can often directly be used for control of the more sophisticated models, while the subsequent model results can be presented simultaneously with the field observations in graphical form by computer-controlled plotters for an immediate evaluation by the investigator.

Mathematical modeling has an advantage which has not yet been used extensively. It enables representation of results in the form of an animated movie by plotting results of successive steps of a computation in graphic form on 35- or 16-mm film. This permits presentation of research results in an understandable manner to a large audience. It is also a tool for the investigator in the understanding of the relationships of transients which do occur. For example, water level gradients, which are not perceptible in nature or in the physical model, can be shown in relation to currents by plotting the water surface in an isometric projection above the plan view with current vectors.

From this presentation, it is clear that the organization of an investigation using mathematical models is difficult, particularly as experience with these models and with related fluid flow models has shown that effective and productive research can be done only with a small group of investigators, where the principal investigator is intimately familiar with all aspects of the investigation. Research "by committee" is highly inefficient and has led to complete failure of certain projects in the computer industry. It is apparent from large model developments in related disciplines that many critical requirements have to be satisfied for the organization and support of an effective and productive research group developing mathematical models. It may be expected that the existing pattern of research and also the relations between academic institutions, governmental research departments, and the field exploration groups will be drastically altered to adjust to the extensive use of this new tool.

It was indicated that modeling of certain physical processes is possible. Consequently, many physical processes can now be studied effectively with mathematical models in a manner such as used in the modeling of the fluid dynamics of the atmosphere and the oceans. The tremendous power of digestion and representation of data by computer methods opens the way for investigations of mass transport in estuaries, circulations and generation of surges and seiches by wind and tides. All these are important in water quality studies.

Up to this part of this discussion, emphasis has been on the physical processes, which have been more accessible for formulation and subsequent modeling. Biological systems are notoriously complex, highly nonlinear, and their interactions not well understood. An important tool has now appeared, namely BIOMOD, which is an interactive computer-graphics system for biological modeling. This system operates on an interactive graphics console comprising a cathode ray tube screen, a tablet, and a keyboard. It allows a user to draw block diagrams of the biological system, each component of which can be defined by another block diagram. The relationships which are presumed by the investigator in the model component can be inserted as differential equations, chemical equations, or data curves. The system allows use of handprinted text or the use of a keyboard for the mathematical expressions and parameter values, etc. The system operates in two phases, a construction phase, in which the user draws and specifies models, and a simulation phase, which simulates the models and outputs results. In the simulation phase the computational programs are written by the computer and subsequently used in the simulation. Graphics results are depicted on the screen during simulation. The investigator controls nearly all action with a pen-like stylus on the tablet. The mathematical models of biological communities of the type described in this report by Dr. Paulik can become operational in a single session. Since the modeling system is interactive, new pathways envisioned by the investigator can be explored very rapidly; also, the influence of coefficients can rapidly be evaluated.

From this discussion it will be clear that mathematical models will become a more powerful tool as time progresses, a tool whose usage we have to learn, but also a tool which we urgently need for solving one of the most threatening problems of our civilization.

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4.4 DISCUSSION by W. H. Espey

Estuaries constitute one of our most valuable and vulnerable natural resources. As the economic value of the estuarine zone rises, and population pressures increase, the conflict between competing uses of the estuaries becomes a vexatious problem. Approximately 30% of the total population live within fifty miles of the coastline of the continental United States, and of this coastline, nearly 85% of the Atlantic and Gulf Coast, and 15% of the Pacific Coast are estuarine (Singer 1969). Yet this same coastal belt represents only 8% of the total land area of the United States (Pritchard 1966). As the entire population call upon and derive some benefit from the estuarine zone, the nation has been forced to recognize that what it has in surplus is now in jeopardy. Increasing conflict over the use of our valuable estuaries has dictated the necessity for comprehensive water quality management of this valuable natural resource.

Water quality models play an important role in this management, as they provide a tool by which quantitative assessment can be made of various water quality control programs and their effect on the marine environment. Numerous management alternatives, such as low flow augmentation, relocation of outfalls, various waste treatment schemes, and even physical modification of the estuary, can be examined with respect to meeting specified water quality standards within the estuary.

All too often, however, the role which the models are to play in the management process is hampered from the outset by a lack of clear definition of the water quality problems which the models are expected to address. Specification of the requirements of the water quality models, that is what the models will be expected to do, is essential in the initial selection process. These requirements will undoubtedly influence the modeling approach. In many cases a slide rule computation will suffice to answer certain questions; however, detailed questions with regard to such things as waste distribution around an outfall, or the effect of a barrier on the water quality conditions in an area of the bay require a more detailed model. Existing models or modeling techniques may be sufficient, however, the development of new techniques might be required. These are the questions which should be resolved early in the course of any modeling endeavor.

A particular aspect of the selection process concerns spatial resolution. In general, models which describe the distribution of a constituent within an estuarine system, while capable of evaluating the effect of a single discharge on the total system, cannot yield detailed information in the immediate vicinity of the discharge. A good example is the evaluation of a thermal discharge into the Galveston Bay system as described in the Case Studies, Chapter VII, Section 5. The models developed as a part of the Galveston Bay Project, utilizing a one square nautical mile (850 acres) spatial resolution, can hardly be expected to describe the mixing zone of the discharge which averages some 650 acres. In order to evaluate the thermal effects near the outfall, a much finer resolution is required. These fine grid models, as they are sometimes referred to, are based on the same physical principles; however, new problems are often encountered. Experience has shown that boundary conditions, stability criteria, source and sink definition, and in a more general sense, solution techniques may well differ in this fine grid environment.

In summary I wish to emphasize that a clear definition of the kinds of problems which the models are expected to address is of paramount importance in the design or selection of the appropriate model. At times users of water quality models have the impression that any model can do everything. Simply stated, a lack of communication often exists between the modeler and the user. If we are to successfully withstand the challenge of resolving the conflict of demands on our estuarine waters, given all the technical and financial limitations, enough cannot be said for a sound foundation of discussion between the primary participants in the modeling effort. In the future we can expect new problems in our estuaries as a result of new waste materials from industry. Increased concern for ecological considerations will probably require the modeling of other constituents such as toxicity and certain heavy metals in the marine environment. This will require investigation of the various sources and sinks that effect the fate of that constituent in the estuary.

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5. REVIEW AND COMMENTS

Arthur T. Ippen

The state-of-the-art of our knowledge on estuarine water movement and quality with its transient features has been in rapid development in the past ten years. While much has been accomplished many more gaps in our knowledge and in our methodology of dealing with estuarine management problems have also been laid bare. With our increased capabilities in the analytical, experimental and computer-based methodologies, progress is substantial and proceeds unabated as more sophisticated demands are placed before engineers and managers by the national community concerned with problems in shoreline and estuarine environments.

The more intensive research activities started more than twenty years ago when the U. S. Corps of Engineers found its design capabilities for proper maintenance of navigation channels in tidal regions severely limited. This was true particularly with regard to the unknown interaction of the saltwater-freshwater flows in estuaries to which the shoaling patterns had been traced. It proceeded through its Committee on Tidal Hydraulics towards the systematic investigation of these phenomena through basic analysis and experimentation on physical models assisted by interested members of the academic community. The fortuitous advent of the computers supplied a vastly increased range of opportunities for extensive analytical studies to these investigators. More detailed solutions of the basic differential equations for tidal and water quality conditions in real estuaries became possible with physical information supplied by hydraulic models and field explorations. Concern with the dispersion of conservative and nonconservative pollutants and with their effects on water quality had developed greatly the range of interest in the governing hydrodynamic aspects of the complex flows in estuaries.

A detailed summary of the state-of-the-art at this time as attempted in this volume seems therefore highly appropriate. The array of contributions by the leading investigators is most impressive not only with regard to their individual summaries but also with regard to the effort made to express alternative viewpoints and to reconcile "interdisciplinary" problems. The wide range of topics covering hydrodynamics, chemical and biological processes and the various modes of the research technologies place the subject of the estuarine water quality analysis beyond the expertise of individuals. Hence, this collective effort by carefully selected professionals was the only feasible way towards a comprehensive review of present-day knowledge. In the opinion of this reviewer, who had the privilege to follow its development, it is a most successful effort and should be most useful to all those active in the field who must be aware of the wider aspects and implications of their particular tasks in the context of estuarine water control.

Limiting the following remarks to the area of this reviewer's interests, a few more specific comments are made on the chapters pertaining to the primary dynamics of the carrier fluids in estuaries, the saline and fresh waters involved in the tidal processes in complex geometric boundaries.

It is fair to say at this point that much of our knowledge in the past in the area of prediction of tidal phenomena in estuaries including the saltwater-freshwater mixing processes was primarily guided by investigations on "Physical Hydraulic Models." The chapter under this title written by my colleague, Dr. D. R. F. Harleman, gives an excellent summary of the analytical premises and of the physical limitations of this methodology of problem-solving in estuaries. Hydraulic models have been built all over the world and have acquired a reputation of general reliability for the solution of specific engineering problems. As long as the predictive capacity pertained to tidal stages and velocities in complex estuaries this confidence level was justified even to the extent of analyzing shoaling trends under verified salinity intrusion patterns. As Dr. Harleman points out, however, severe restrictions exist with regard to the utilization of hydraulic models for pollutant dispersion studies in view of the usual distorted scales employed. The analytical conditions for dispersion in the nonsaline portion of the estuary are different from those in the salinity intrusion length. It is most important to realize this limitation when conducting pollutant dispersion experiments; nevertheless comparative studies of dispersion in three-dimensional models can still serve useful purposes since, except for expensive field studies, no other means are at hand to predict dispersion coefficients which are also necessary for numerical models. However, it is clear that mathematical modeling with its more flexible possibilities of changing boundary conditions will replace the physical models in estuaries of simple geometry where one-dimensional approaches are deemed adequate. The value of Dr. Harleman's Chapter V on "Physical Hydraulic Models" lies in its complete and sound examination of the analytical principles for such models and of the limitations inherent in the impossibility of meeting all similarity criteria within the economic restraints applicable to model construction and operation. This chapter must be consulted when hydraulic models are being planned so that their probable usefulness for the solution of the respective problems is apparent from the outset.

Chapter II on "Hydrodynamic Models" is divided into three parts successively proceeding from the complex cases of three-dimensional and two-dimensional models treated by Dr. Pritchard to the one-dimensional models dealt with by Dr. Harleman. This sequence corresponds to the progressive ability to deal with mathematical modeling as the number of dimensions considered is decreased, but also to the increasing inability to represent mathematically all the physical factors adequately which usually govern the tidal and dispersion phenomena in estuaries. Research in the area of hydrodynamic modeling for practical reasons is proceeding therefore in the opposite direction replacing bulk properties of the one-dimensional models with their more sophisticated components which represent more realistically the details of the physical system in the two- and three-dimensional models. This research is presently most active and, while difficult, will yield increasingly useful returns as computational techniques and capacities are developed and more competently exploited in addition to more exhaustive field studies to define necessary inputs to the two- and three-dimensional schemes. Dr. Pritchard sets forth very clearly the various procedures and assumptions needed to make the three-dimensional set of equations more amenable to solution. In particular, attention is given to the definition of the eddy-diffusivities and of the eddy-viscosities, which have been determined numerically only for a few isolated instances. Analytical determination of these coefficients in salinity intrusion regions with various degrees of mixing are not available. Numerical solutions for three-dimensional mathematical models of real estuaries are concluded to be still beyond practical attainment.

The various approaches to two-dimensional models are also discussed in detail by Dr. Pritchard based on the introduction of vertically averaged "effective" diffusion coefficients for the two horizontal directions. These are different in value from the three-dimensional coefficients and again are required to be known for a numerical solution. This dilemma is shared to a lesser degree by the scheme proposed by J. J. Leendertse, but also this scheme requires prior knowledge of alternate local diffusivities as vertically averaged coefficients. Specific applications of two-dimensional models covering tidal and salinity characteristics are not given. It should be feasible, however, to cope numerically with two-dimensional models at least in cases where the estuary is vertically nearly homogeneous in velocity and salinity.

Dr. Pritchard appropriately calls special attention in both of his sections to the presence in the dynamic equations of the isobaric gradients in the salinity intrusion zones. Their numerical values are shown to be most significant as illustrated by sample calculations and comparisons with surface gradients.

The "One-Dimensional Mathematical Models" which so far have had considerable practical use are described in careful detail by Dr. Harleman in Chapter II. Since many schemes have been developed and are used, specific attention is focused on the definitions of velocity and salinity as averaged in various schemes over time and space. Three-dimensional mixing processes are not neglected but are incorporated in the redefined longitudinal dispersion coefficient. The independent variables are reduced to the tidal velocity, the cross-sectional area and the dispersion coefficient, all of which may be functions of longitudinal distance and time. The determination of the redefined dispersion coefficients for the one-dimensional case has yielded practical values from theory for uniform density sections and from salinity measurements for the intrusion regions. Tidal velocities are readily computed from numerical schemes while the necessary cross-sectional information is available from surveys and is used to divide the estuary into appropriate sections for numerical computation. A number of specific solutions are reviewed from the simple case of the uniform estuary for which extensive experimental material exists to the more complex cases.

Emphasis is rightfully given by Dr. Harleman to the solution of the real time mass transfer equations as being most accessible through theoretical and practical determinations of the dispersion coefficients. The difficulties encountered with suitable dispersion coefficients in mathematical models under nontidal advective conditions are effectively illustrated by examples. It is concluded that the real time mass transfer equation offers the best approach to future analysis when finite-difference techniques are used in computer solutions and results in most realistic representations of dispersion phenomena. Since the major problems of pollution center on the dispersion of nonconservative substances and on chemical-biological interaction in estuaries, this aspect seems most promising for future progress in research.

In conclusion it may be stated that this entire estuarine state-of-the-art study as represented by this timely collection of reviews by different authors fills an important function in our still continuing search for better predictive as well as monitoring methods. Undoubtedly major manmade changes in the estuarine environments of this country will be forthcoming in the future. Their effects on the ecology can hopefully be assessed with greater confidence. Research as reviewed in this volume will contribute to our awareness of the consequences of such changes and will help to prevent unexpected and possibly irreparable damage. May this volume also stimulate the urgently needed support for expanded research from all agencies concerned so that present momentum in interest and knowledge may not be dissipated. We have a long road ahead.

CHAPTER X

CONCLUSIONS AND RECOMMENDATIONS

Throughout this report, conclusions have been drawn and discussed concerning the various aspects of estuarine water quality modeling. Recommendations have been made concerning the research required to remedy present.deficiencies in the models and to develop more advanced models capable of treating the complexities of estuarine water quality. The background development and discussion context are basic to their interpretation, and therefore the reader is referred to the individual chapters for the recommendations and conclusions appropriate to that topic. Nevertheless, it is of value to attempt a compilation and summary in this section.

As in the preceding sections of this report, we continue to discuss separately the hydrodynamic processes and the reaction processes. As emphasized below, however, in a specific estuary, the relative importance of hydrodynamics and kinetics must be ascertained in applying or evaluating the adequacy of a model.

1. CONCLUSIONS

1.1 ESTUARINE HYDRODYNAMIC MODELS

(1) The adequacy of present hydrodynamic models is dictated to a large extent by their dimensionality. The present state-of-the-art of one-dimensional hydrodynamic models is well advanced, and good results may be obtained if one employs "real time" computational techniques especially in the constant density region. The existing theory and computational techniques for vertically averaged two-dimensional hydrodynamic models (particularly appropriate for broad, shallow estuaries) appear to be adequate although in many instances the application may have been less than state-of-the-art. The theoretical principles underlying the vertical plane (laterally averaged) two-dimensional models as well as the general three-dimensional models are generally well-in-hand. However, the solution techniques are not advanced at all due to the necessity for representing gravitational circulation, which requires solution of the coupled equations of motion and salt transport. Some similarity solutions have been obtained for the steady-state two-dimensional vertical plane model.

In each case, the relative importance of the various terms in the momentum balance must be ascertained. One term in particular, the horizontal pressure gradient due to varying density, is often omitted, yet appears to be important in many estuaries. Inclusion of this term may also present computational difficulties as it requires simultaneous solution for at least the salinity distribution.

(2) The greatest weakness of present hydrodynamic models is the treatment of the eddy diffusivities and dispersion coefficients, particularly within the salinity intrusion region of estuaries. Present methods rely on measured data (usually salinity), adjusting the dispersion coefficients so that the model reproduces the measured data. The effects of the estuarine environment and physiography on the dispersion are virtually unknown, so the predictive capabilities of the model are severely limited. A theoretical or quasi-theoretical foundation is needed for the calculation of the dispersion coefficients on the basis of external influences (wind stress, waves, etc.) and the gross hydrographic parameters of the estuary.

The meaning and magnitude of the diffusion-dispersion coefficient is highly dependent upon the spatial and temporal averaging employed in deriving the fundamental equations. For the one-dimensional case, dispersion coefficients for a "real time" model (which considers the tidal motion) may be estimated sufficiently well in the uniform density region by an extension of the Taylor-Elder formula, although within the salinity intrusion region dispersion coefficients must be determined empirically. For a one-dimensional "non-tidal advective" model (which considers only the freshwater through-flow), dispersion coefficients can only be determined empirically. In the application of one-dimensional non-tidal models to some estuaries, the constituent profiles may not be especially sensitive to the dispersion coefficients, so that accuracy in their determination is not critical. It has been suggested that for long-term estuary studies, both real time and non-tidal advective models be developed, using the former to calibrate the latter.

(3) Although one-dimensional and vertically averaged two-dimensional models have been employed in numerous estuaries, there is a sparsity of thorough verification. The usual practice is to verify the model by comparing the tidal height and phase at various points in the estuary. It appears, however, that this is an inadequate measure of how well the model predicts currents in the estuary. Although the question of field programs and data collection lies somewhat outside an assessment of estuarine modeling, nevertheless this assessment requires adequate observations in real estuaries in order to identify the relative importance of the hydrodynamic influences. For many types of estuaries, such observational data are lacking.

1.2 ESTUARINE WATER QUALITY MODELS

(1) It is concluded that as a general rule, the modeling of the hydrodynamic transport of a constituent in an estuary is much further advanced than the modeling of its reaction kinetics. This must be qualified according to the particular constituent and circumstance: there are important problems which are hydrodynamically dominated, just as there are constituents whose reaction kinetics are well established. However, the most commonly unsatisfactory aspect of present water quality models is the specification of the source and sink terms.

(2) Many of the physico-chemical processes affecting the concentration of parameters lack adequate formulation, in that not only are the coefficients unknown, but the forms of the reactions are poorly established. These include sedimentation and deposition of particulate matter, nonlinear reaction kinetics, surface exchange of gaseous constituents, and chemical and biological reactions.

(3) Many of the important water quality parameters behave in a highly coupled manner, e.g., the species of nitrogen. Specification of the reactions involved as well as the formulation of computational techniques for treating general nonlinear interdependencies ("feedforward" and "feedback" reactions) are inadequate at the present.

(4) Small-scale problems such as distributions in the locality of a discharge, thermal discharges in the initial and intermediate scales, nearshore disposal, peripheral embayments, etc., pose modeling problems for which grosser models as applied to the entire estuary are not sufficient. These problems require refinement in both the transport and reaction kinetics, and, due to the fine temporal and spatial detail, also may impose extreme demands on the solution procedures.

(5) Modeling of the relation of water quality and the estuarine biota is not well-advanced at all. Models of phytoplankton production, of nitrogen cycling, and of gross ecological parameters (species diversity, bioassays of toxicity) have been attempted, but presently these are at best experimental. Only recently have Michaelis-Menten type kinetics been utilized in estuarine and oceanic models. Models of finfish population dynamics, on the other hand, have a longer history and, hence, a somewhat more advanced development.

1.3 UTILITY OF PHYSICAL MODELS

(1) The greatest potential value of the physical model is its ability to represent three-dimensional systems, whose complexity precludes conventional analytic techniques. Despite the lack of complete similitude, due to vertical distortion, useful results can be obtained by comparative tests of alternative schemes.

(2) It must be borne in mind that estuarine physical models are Froude-scaled and therefore, if properly verified, are capable of representing Froude-type phenomena such as tidal currents, momentum entrainment and gravitational circulation. On the other hand, local currents and turbulent eddies which are not Froude-type phenomena are not necessarily well-represented in physical models. For this reason, there is considerable distortion of diffusive processes in the physical model that makes its utility in quantitative concentration distribution studies dubious.

The validity of extrapolating dye releases in the physical model to the real estuary is presently in doubt, due not only to questions of similtude, but to questions of measurement in the physical model. Inadequate verification of such releases prevent a thorough appraisal of the model's utility in this case.

(3) Modeling of complex reactive constitutents and coupled reactants at present is not possible with the physical model.

(4) From a qualitative standpoint, the physical model possesses an excellent demonstration capability for the visualization of flow patterns and resultant concentration distributions. With the formidable problems of communicating the results of water quality investigations to a nontechnical audience, this capability should not be underrated.

1.4 SOLUTION TECHNIQUES

(1) In general, analog computers are falling into disuse relative to their digital counterparts. This appears to be due to the unwieldiness and lack of versatility of the analog computer as well as the increased availability and ease of programming of digital computers.

Both have advantages and disadvantages, and the choice of a particular technique in the final analysis is contingent upon the characteristics of the equations, the intended use of the model results, required accuracy, available resources, experience of the personnel, and similar criteria which are really ancillary to the problems of estuarine water quality modeling.

(2) The technique of finite-difference approximations is the most popular and promising method of solution to the complex partial differential equations which constitute estuarine water quality models. In applying this technique, consideration should be given to the problems associated with the approximations, for instance, accuracy and stability of the computation, convergence questions (when appropriate), numerical distortion of the transport and reactive processes, etc., in order to ensure the validity of the results. In many past numerical studies, these considerations have been disregarded.

1.5 APPLICATIONS

(1) For any particular estuarine quality problem, a preliminary effort should be devoted to determining the model appropriate to that problem. The features of an estuarine system should be considered in determining the spatial dimensionality, temporal and spatial refinement, and so on, of the model. All too often, the physical integrity of the model is sacrificed for simplicity or expedience. On the other hand, models have been constructed which are far too detailed for the problem under investigation. Similarly the relative influence of the hydrodynamic and the kinetic terms should be investigated, so that the model employed is neither overly complex nor superficial.

(2) Utility of models in evaluating both the effects of streamflow modification (including augmentation, regulation, and upstream diversion) and the effects of physiographic modification is basically limited by the predictive capability of the hydrodynamic models. In the case of the former, many estuaries amenable to a one-dimensional treatment have been modeled with various magnitudes of inflow and the results employed in management studies. Very little work using more complex mathematical models has been performed. Physiographic alterations have been studied almost exclusively with physical models.

2. RECOMMENDATIONS FOR FUTURE RESEARCH

The distinction should be recognized between a conceptual problem and a computational problem. Much work is required in strengthening the conceptual aspects of estuarine models, whereas available computational techniques, employed rigorously, are in many cases sufficient.

Emphasis in future research should be placed upon the source and sink processes of specific water quality parameters. There are, of course, important aspects of estuarine hydrodynamics which require continued study, but an increased effort is needed in the study of the various reactions in order to produce models adequate for treating estuarine water quality problems. Such work will not necessarily be strictly of a modeling nature. Rather, laboratory and field studies of the processes will also be required. The results of these studies, however, should be capable of incorporation in estuarine models.

2.1 HYDRODYNAMIC MODELS

(1) Research is required in establishing methods whereby the dispersion coefficients (or eddy diffusivities, as the case may be) may be predicted from hydrographic and environmental factors.

(2) Development should be undertaken of models capable of representing the vertical dimension, viz. laterally averaged two-dimensional models and three-dimensional models. These models must represent the hydrodynamic effects of density gradients, and may therefore require the development of appropriate computational procedures.

(3) In all hydrodynamic models, the importance of the pressure gradient due to density (i.e., due to the internal slope of the pressure surfaces) must be considered and, if necessary, included in the model.

2.2 WATER QUALITY MODELS

(1) Work is needed in the study and mathematical delineation of the reactions to which estuarine constituents are subjected. Clarification of the processes affecting dissolved oxygen is required, as well as modeling of other parameters, e.g., sulfates and sulfites, heavy metals, carbon dioxide, particulate matter, and so on. The phenomenon of gaseous diffusion through the surface and its dependence upon physico-chemical features of the estuary require study.

(2) Research is needed into the behavior and modeling of coupled reactions. In particular, the problem of general nonlinear coupled reactions (with feedforward and feedback dependencies) requires investigation from both a physical and a computational standpoint.

(3) Research should be pursued in the modeling of biota and their interaction with constituents of estuarine water. This ranges from models of phytoplankton populations through models of the higher trophic levels up to fishery resource models.

(4) Models are required that are capable of representing the local effects of a discharge in the nearshore environment. These will encompass both the hydrodynamics and kinetics of such a discharge. Considerable effort may be required in developing suitable computational techniques for this kind of problem. Physical models may also prove to be useful here, if accompanied by a rigorous analysis of similitude requirements.

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27 Abstract

This report constitutes a technical review and critical appraisal of present techniques of water quality modeling as applied to estuaries. Various aspects of estuarine modeling are treated by a selection of scientists and engineers eminent in the field, and these essays are supplemented by discussions from technical conferences held during the course of the report's preparation. Topics discussed include mathematical models for estuarine hydrodynamics, water quality models of chemical and biological constituents, models of estuarine temperature structure, and the use of physical models in estuarine analysis. Also included is a review of solution techniques, viz. analog, digital and hybrid, a brief survey of estuarine biota and biological modeling, and a collection of case studies reviewing several estuarine modeling projects. Conclusions about the existing state of the art of estuarine modeling and recommendations for future research by EPA are summarized in the final chapter.

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